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⑥ COMPUTER CALCULATIONS OF ROCKET
ENGINE COMBUSTION PROPERTIES,

⑩ by

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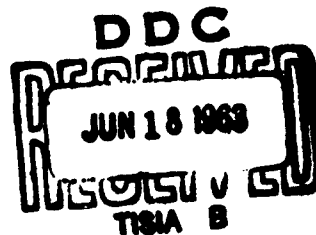
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⑰ NA
⑱ is
⑲ master's
thesis

G.C.

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I can remember as a boy in Junior High School, I dreamed of being a Rocket Engineer. To the United States Air Force, to the University of Wyoming, and especially to Professor Robert A. Wheasler of the Department of Mechanical Engineering, I am deeply grateful for having the opportunity to study the subject of rocket propulsion. For the opportunity to write this paper, I will forever be in debt to all who have offered assistance.

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TABLE OF CONTENTS

CHAPTER	PAGE
I. INTRODUCTION	1
II. HEAT OF REACTION (ΔH_r)	3
III. CHEMICAL EQUILIBRIUM AND THE EQUILIBRIUM CONSTANT.	6
IV. CALCULATION OF ADIABATIC FLAME TEMPERATURE	15
V. RESULTS OF CALCULATIONS.	33
BIBLIOGRAPHY	45
APPENDIX	47
1. Solution of Simultaneous Linear Equations	48
2. Gas Tables from NACA 1037	57

LIST OF TABLES

TABLE	PAGE
I. Combustion Program in Matrix Form.	22
II. First Computer Program	29
III. Second Computer Program.	32
IV. Results of Calculations For O/F Ratio of (0.5) and 23 Atmospheres	35
V. Final Results of Calculations Combustion Pressure 23 Atmospheres	38
VI. Final Results of Calculations Combustion Pressure 20 Atmospheres	38
VII. Results From First Program	41
VIII. Results From Second Program.	44

LIST OF FIGURES

FIGURE		PAGE
4-1.	Interpolation for Adiabatic Flame Temperature.	27
5-1.	Graphical Interpolation for Combustion Flame Temperature.	39
5-2.	Graphical Results for Liquid Hydrogen and Liquid Oxygen.	40

NOMENCLATURE

The following symbols are employed in the derivations of this thesis.

<u>Symbol</u>	<u>Explanation</u>
A_1	Total number of atoms of a particular species in the reactants.
a_1	The number of atoms of a particular species contained in a product of combustion.
a_j	The stoichiometric coefficient in the equilibrium equation.
(a/G)	Mole fraction of species a.
$(a/G)P$	Partial pressure of species a.
C	Centigrade temperature scale.
CONV	Convergence.
Cal	Calorie.
C_p	The value of specific heat measured at constant pressure.
C_v	The value of specific heat measured at constant volume.
CH2	C_p value for hydrogen at some T.
CH2A	C_p value for hydrogen at $T + 100$ K.
F	Fahrenheit temperature scale.
G, g	Gibb's free energy function.
G	Total number of moles when used in the equations of combustion.
gmole	Gram mole.
H, h	Enthalpy.
Hf	Heat of formation (chemical).
Hr	Heat of reaction (chemical).
H2	Enthalpy of hydrogen at T.

NOMENCLATURE (continued)

<u>Symbol</u>	<u>Explanation</u>
H2A	Enthalpy of hydrogen at T + 100 K.
H2S	Enthalpy of hydrogen at 298.16 K.
K	Kelvin temperature scale.
Kcal	One thousand calories.
Kp	Equilibrium constant based on partial pressure.
k	Isentropic exponent (C_p/C_v).
L	work other than expansion work.
Log	Naperian logarithm.
M	Molecular weight.
m	Mass.
N	Number of moles.
n_1	The number of moles of a product of combustion.
O/F	Oxidizer/fuel molar ratio.
P, p	Pressure.
PS	Combustion pressure (atmospheres).
PK1	Logarithm value of Kpl at some T.
PK1A	Logarithm value of Kpl at T + 100 K.
Q	Thermodynamic heat.
Ru	Universal gas constant ($1.98718 \frac{\text{Cal}}{\text{gmole-K}}$).
RS	Fractional value between hundreds of degrees.
S, s	Entropy.
S	Molar ratio (oxidizer/fuel).

NOMENCLATURE (continued)

<u>Symbol</u>	<u>Explanation</u>
T,t	Temperature degrees absolute.
Tc	Adiabatic flame temperature.
TOLER	Tolerance level for the matrix solution.
U,u	Thermodynamic internal energy.
V,v	Volume.
X_i	Error function of substance i.
(3,7)	(Row 3, Column 7) of the matrix.
(2:148)	(Reference 2: Page 148)

CHAPTER I

INTRODUCTION

A rocket engine is a device for converting the thermochemical energy of one or more propellants into exhaust jet kinetic energy. The term propellant is applied to any material, solid or liquid, consumed in the rocket motor for producing high-pressure, high-temperature gases. It is generally assumed, and there is some evidence to support the assumption, that, under the pressure and temperature occurring in a rocket-motor combustion chamber and nozzle, the chemical reaction takes place under conditions which approach chemical equilibrium. Accordingly, in the ensuing discussions the thermodynamic properties of the gas flowing through the rocket motor are assumed to be those from thermochemical equilibrium calculations.

(1:426)*

↙ The scope of this paper ~~will be~~ limited to the equilibrium calculations of combustion products and the resulting adiabatic flame temperature. The problem of attempting to determine the equilibrium constituents as the gases progress through the rocket nozzle ~~will not be attempted at this time although this author realizes the very pronounced problem which exists.~~ Jo p. 2

As the static temperature decreases during the systematical progression of the gases through the nozzle, the molecules of the propellant which have dissociated due to the high temperature in the combustion chamber tend to reassociate. In a basic rocketry problem frozen flow is assumed, that is, the equilibrium combustion of the

* Numbers in parentheses refer to items in the bibliography and the related page number.

1

gases in the combustion chamber is unaltered during the expansion process in the nozzle. (1:436) In the condition of equilibrium flow the equilibrium composition corresponding to the local conditions of pressure and temperature is obtained in each section of the nozzle. The preceding statements correspond to the two extreme cases of frozen or equilibrium flow. In the case of real flow, at a temperature often exceeding 3000 K near the chamber, reactions of recombination take place. (2:179) However, the residence time in the nozzle is very small and these reactions may not have sufficient time for completion. Equilibrium flow, therefore, is not obtained and the real flow is situated at some intermediate point between the two extreme cases.

Before the age of electronic computers, the problem of calculating the combustion properties of a rocket engine was very tedious and almost impossible to solve. Since the present day engineers have access to the electronic computers, it is only fitting that a thesis be presented in a form illustrating the solution of combustion problems by use of the electronic computers.

~~The following presentation is~~ a solution of a relatively simple combustion problem consisting of only six products of combustion. ^{is presented by} By ~~simply~~ understanding and following the illustrated procedures a problem consisting of any number of products of combustion may be computed and solved to any desired degree of accuracy.

CHAPTER II

HEAT OF REACTION (ΔH_r)

The energy released or absorbed in a chemical reaction, under the condition that the products are returned to the initial temperature of the reactants, is defined as the Heat of Reaction. If the reaction takes place at constant pressure, the heat of reaction is equal to the change in enthalpy during the reaction, i.e., $(H)_{\text{products}} - (H)_{\text{reactants}}$. Of course, these enthalpy values must include the energy associated with the chemical bonds of each substance as well as its thermal energy which is due to the random motion of the molecules. (4:1)

The heat of reaction at constant pressure is related to the heat of reaction at constant volume by the following thermodynamic relationships

$$dq = du + pdv = dh - vdp = dH_r \quad (1)$$

The internal energy (U) for an ideal gas is a function of temperature only. From this fact it is possible to make the assumption that for an ideal gas, the finite difference of internal energy (ΔU) at constant pressure is equal to the same value at constant volume, which defines

$$(\Delta U)_p = (\Delta U)_v \quad (2)$$

However

$$(\Delta H_r)_v = \Delta U + \cancel{P\Delta V}^0 \quad (3)$$

and

$$(\Delta H_r)_p = \Delta H - \cancel{V\Delta P}^0 \quad (4)$$

Since by definition

$$H = U + PV \quad (5)$$

then

$$\Delta H = \Delta U + \Delta(PV) \quad (6)$$

on rearranging

$$\Delta U = \Delta H - \Delta(PV) \quad (7)$$

Then by substitution

$$(\Delta H_r)_v = (\Delta H_r)_p - \Delta(PV) = (\Delta U)_p = (\Delta U)_v \quad (8)$$

which can be written as

$$(\Delta H_r)_v = (\Delta H_r)_p - (\Delta n_{\text{gas}}) RT \quad (9)$$

Standard Heat of Formation is the heat of reaction when a compound is formed from its elements in their standard state. The standard state of an element is its stable form at a temperature of 298.16 K or 25 C and a pressure of one atmosphere. The standard state is sometimes referred to as being 0 C and one atmosphere. The standard-state temperature is really artificial, for, if the reaction were to take place isothermally, it would require a perfect heat sink which removes heat from the system as fast as it is liberated by the chemical reaction.

When a substance is combined with oxygen the heat of reaction is called the heat of combustion since the reaction is one in which the oxygen is the oxidizer. The formation of carbon dioxide from its elements in their standard state is as follows



Here the carbon must be in the graphite state since that is the stable form of carbon at 25 C, likewise the oxygen and the carbon dioxide must be in the gaseous state. Under these conditions the heat of reaction is the standard heat of formation of CO_2 . In this case

the heat of reaction can also be called the heat of combustion.

The sign associated with the heat of reaction is an indication as to whether the reaction is endothermic (takes up heat) or exothermic (gives off heat). In this country normally a minus or negative sign is associated with an exothermic reaction. This convention is not true all over the world. An easy way to determine which convention is used for any particular set of tables is to check the heat of formation of water. Water will always have an exothermic heat of formation and from this, the correct sign convention can be determined for the remaining substances.

CHAPTER III

CHEMICAL EQUILIBRIUM AND THE EQUILIBRIUM CONSTANT

There are several different ways of defining and expressing the equilibrium constant. For example, depending upon the circumstances, the equilibrium constant can be based on concentrations, activities, fugacities, or partial pressures of the constituents present in the equilibrium mixture. In situations where the perfect gas law is closely followed by the constituents of the mixture, the equilibrium constant based on partial pressures is the most useful, i.e., the most easily applied.

An arbitrary thermodynamical system which is separated from its surroundings by a control surface which is a perfect thermal insulator, will now be considered. It is desired to determine from the thermodynamic characteristics of the system whether or not the system is in equilibrium or undergoing a spontaneous change of state. As a first step in the consideration of the aforementioned problem, it is necessary to determine what information can be derived by applying the first and second laws of thermodynamics to the system. The only information furnished by the first law is that one type of energy can be converted into another, and the ratio of the conversion is constant. The first law gives no information regarding the direction in which an energy transformation will proceed. As far as the first law is concerned, it is possible for the conversion to proceed in any direction that is permitted by the constraints imposed on the thermodynamic system. Thus the first law gives no information whatsoever regarding either the spontaneity or the

direction of a physical or chemical process. (2:529)

The second law established the principle that it is impossible to take heat from a system and convert it into work without simultaneous changes occurring in the system or in its environment. From the second law it is learned that only for a reversible adiabatic (isentropic) process is the entropy constant. From the entropy principle it is deduced that the only changes of state (processes) that are possible are those which produce an increase in the entropy of an isolated system. The second law gives no information indicating whether or not a process will take place if the constraints imposed on the system do allow the entropy of the system to increase. Thus it is seen that neither the first nor the second law provides the information for determining (1) whether a thermodynamic system is in equilibrium, and (2) if a spontaneous change of state can occur in a thermodynamic system.

The internal energy (U) of a thermodynamic system is analogous to the potential energy of a dynamic system. A dynamical system which is at rest can be set into motion spontaneously if the constraints imposed on it permit the potential energy of the system to diminish. The potential energy of the system tends to convert itself spontaneously into kinetic energy. Studies show that, assuming conditions permit, a dynamical system will be in equilibrium when its potential energy is a minimum. It is a fundamental principle of dynamics that a dynamical system tends to attain the state where its potential energy is a minimum, subject, of course, to the geometrical constraints imposed on the system. Thus, the internal energy (U) of a thermodynamical system, if permitted to do so, will be transformed into other forms of energy

having a nonpotential energy nature, until the equilibrium condition for the system is attained. Hence, a spontaneous change of state can take place in a thermodynamic system only if it occurs in the direction which tends to make the internal energy of the system a minimum, and the system will not be in equilibrium until the minimum value of U is attained. Hence, one fundamental principle that gives spontaneity of a process is that the process must proceed in the direction that will result in the U of the system proceeding to a condition of U -min.

From the second law the change of state for an isolated thermodynamic system must result in an increase in the entropy of the system. Since the entropy of the system must increase, the equilibrium condition will be attained only when no further increase in entropy is possible, that is, when the entropy of the system is a maximum, subject to the constraints imposed on it. Hence, a natural process can proceed only in the direction allowing S of the system to approach S -max.

From the preceding it follows that the necessary and sufficient conditions for a thermodynamical system to be in equilibrium are: (1) its internal energy must be a minimum, and (2) its entropy must be a maximum. Hence, a spontaneous process is possible only if the change of state can proceed so that the conditions of $U \rightarrow U$ -min and $S \rightarrow S$ -max are satisfied.

The free-energy denoted by G (Gibbs Function) is defined by

$$G = H - TS = U - TS + PV \quad (11)$$

Since H , U , T , and S are thermodynamic point properties, the free-energy function G is likewise a point property. Hence, a finite change, such as ΔG depends only on the final and initial states of the system.

The exact differential dg is given by

$$dg = du - tds - sdt + pdv + vdp \quad (12)$$

Combining the first and the second laws of thermodynamics results in the following familiar equations

$$t ds = dq = du + pdv = dh - vdp \quad (13)$$

One very important statement which is quite often overlooked by the student of thermodynamics is that these equations are based on a pure substance, that is, a substance which is chemically homogeneous and fixed in chemical composition. If the state of the system is such that no chemical reaction can occur without an external stimulus, then the system is in complete (mechanical, thermal, and chemical) equilibrium. When in such a state, the system is chemically homogeneous and invariant; so it is a pure substance and the preceding relationships will apply. However, when a spontaneous chemical reaction occurs it is an irreversible process of a nonpure substance and the equations become (6:482)

$$t ds > du + pdv \quad (14)$$

or

$$t ds > dh - vdp \quad (15)$$

In the statement of the first law for a closed system, where

$$du = dq - dw \quad (16)$$

it is considered that dw is equal to $pdv + dL$, and defines dL as work other than expansion work; the $t ds$ equations for a chemical reaction may then be written as

$$t ds = du + pdv + dL \quad (17)$$

or

$$tds = dh - vdp + dL \quad (18)$$

The free-energy equation is then stated as

$$dg = du + pdv + vdp - tds - sdt \quad (19)$$

Then substituting for tds from equation (17)

$$dg = du + pdv + vdp - (du + pdv + dL) - sdt \quad (20)$$

which results in

$$dg = vdp - sdt - dL \quad (21)$$

In the special case where $dp = 0$ and $dt = 0$, the finite change in free-energy for such a process is denoted by

$$(\Delta G)_{tp} = (G_2 - G_1)_{tp} = -\Delta L \quad (22)$$

This equation shows that the change in the free-energy function $(\Delta G)_{tp}$ represents the maximum (nonexpansion) useful work obtained from a constant temperature and pressure process. It also shows that, for a process conducted so that $dp = 0$ and $dt = 0$, the useful work ΔL is equal to the decrease in the value of the free-energy function.

The free-energy function finds its principal use in establishing the criteria for predicting the equilibrium of chemical and physical processes. For a system that is in equilibrium at a given temperature and pressure, the value of the free-energy function is a minimum. Moreover, for a process to take place spontaneously without change in temperature and pressure, the corresponding change in the free-energy function must be negative. Hence, for a spontaneous change (with $dp = 0$ and $dt = 0$)

$$(\Delta G)_{tp} = (G_2 - G_1)_{tp} < 0 \quad (23)$$

The foregoing provides a criterion for the possible existence of equilibrium. If $(\Delta G)_{tp} = 0$, a spontaneous change of state is impossible. The foregoing shows that, if the free-energy function at a second state (state 2) is less than it is in the initial state (state 1), the system must eventually pass to state 2. Thus the change in the free-energy function is a measure of the tendency of a system to change its state; that tendency is called the escaping tendency.

From the discussion of the free-energy function the following conclusions may be drawn.

1. The only chemical reaction that can proceed spontaneously are those for which the free-energy function decreases.
2. If a chemical reaction gives no change in the free-energy function, then the reaction is in the equilibrium state.
3. Since the direction of a chemical reaction depends on the concentrations of the chemical species involved, the values of the free-energy function for the different species are related to their concentrations.
4. If the reactants in a chemical process cannot form the desired products by a given isothermal process, they cannot form them by any other process, because the change in the free-energy function is independent of the path since it is a property.

When H_2O and CO_2 and other products of combustion are subject to temperatures of 4300 F and higher they tend to dissociate in a manner and to a degree determined solely by the temperature of the mixture. When the products of combustion dissociate, heat is absorbed, which decrease the energy available to accelerate the combustion gases

through the rocket engine. Dissociation is a reversible reaction, that is, one that will go in either direction. In any mixture of products and reactants both dissociation and combustion are constantly occurring. When the rate of dissociation equals the rate of combustion the reaction is in chemical equilibrium and an equilibrium constant exists.

In the general chemical reaction



A, B, C, D represent various substances and a, b, c, d represent the corresponding stoichiometric coefficients. (9:498)

For this example it will be assumed that all the substances involved represent ideal gases. The double arrow indicates that when equilibrium is achieved each substance will be present in a certain amount, and each substance will exist at its partial pressure. As previously stated for a system to be in equilibrium dL must equal 0, that is, no work is being done. From this, equation (21) becomes

$$dg = vdp - sdt \quad (25)$$

which for a isothermal process reduces to

$$dg = vdp = \frac{RuT}{p} dp \quad (26)$$

Then upon integrating from p^0 to p and g^0 to g , equation (26) becomes

$$g - g^0 = RuT \log \frac{p}{p^0} \quad (27)$$

By letting subscript zero refer to standard conditions at one atmosphere

$$g - g^0 = RuT \log p \quad (28)$$

where p is in atmospheres.

From the mixture of gases as given in the previous general

equation (24), the following can be written

$$g_A - g_A^0 = RuT \log p_A \quad (29)$$

$$g_B - g_B^0 = RuT \log p_B \quad (30)$$

$$g_C - g_C^0 = RuT \log p_C \quad (31)$$

$$g_D - g_D^0 = RuT \log p_D \quad (32)$$

Now by writing an expression for the change in Gibb's free-energy function as the reaction goes to completion, that is, starting with reactants A and B and ending with products C and D and since

$$\Delta G = G \text{ products} - G \text{ reactants} \quad (33)$$

then

$$\Delta G = cg_C + dg_D - ag_A - bg_B \quad (34)$$

Substitution in the pressure equations (29) through (32), gives

$$\begin{aligned} \Delta G &= cg_C^0 + c RuT \log p_C + dg_D^0 + d RuT \log p_D \\ &\quad - ag_A^0 - a RuT \log p_A - bg_B^0 - b RuT \log p_B \end{aligned} \quad (35)$$

However, ΔG^0 is defined as

$$\Delta G^0 = cg_C^0 + dg_D^0 - ag_A^0 - bg_B^0 \quad (36)$$

and equation (35) then reduces to

$$\Delta G = \Delta G^0 + RuT \log \frac{p_C^c p_D^d}{p_A^a p_B^b} \quad (37)$$

When the reaction is in equilibrium ($\Delta G = 0$), and since ΔG^0 is a constant and RuT is a constant, the quantity

$$\log \frac{P_C^c P_D^d}{P_A^a P_B^b} \quad (38)$$

must be equal to a constant which is defined as

$$\log K_p \quad (39)$$

This results in the following equality

$$K_p = e^{\frac{-\Delta G^\circ}{RT}} \quad (40)$$

where K_p is the equilibrium constant expressed by the partial pressures of the combustion gases.

For this paper no attempt will be made to consider the equilibrium constant which is expressed in values of concentrations, activities, or fugacities.

CHAPTER IV

CALCULATION OF THE ADIABATIC FLAME TEMPERATURE

All methods for determination of the adiabatic flame temperature and the composition of the combustion products are based on two principles: the First Law of Thermodynamics and the Law of Conservation of Mass. These two principles when used in conjunction with experimentally determined chemical equilibrium data, yield a system of simultaneous equations in terms of the gas composition. The various methods of determining the gas composition differ in the manner in which the simultaneous equations are set up and solved.

By applying the First Law of Thermodynamics and the Law of Conservation of Mass to a chemical reaction it is possible to define the term Adiabatic Flame Temperature. Assuming that the chemical reaction is at constant pressure and adiabatic, and that there is no shaft work performed, the First Law of Thermodynamics states that the enthalpy of the reactants at their temperature prior to the reaction (T_b) is equal to the enthalpy of the products of the reaction at the flame temperature (T_c). Here the enthalpy must include the chemical energy of the molecules of each specie as well as their energy due to random motion, since changes in internal energy occur as a result of the rearrangement of the molecules during reaction.

The Law of Conservation of Mass applied to a chemical reaction requires that the number of atoms of each element remain constant. For example, the number of atoms of a single element in the products after the reaction must be equal to the number of atoms of the same element

in the reactants prior to the reaction, and the same is true for all other elements. Thus in accordance with the definition of a mole, it can be said that the number of atoms of any particular species is constant.

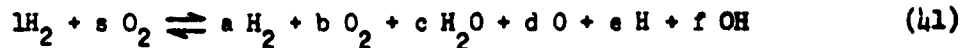
With the aforementioned laws of natural response, the necessary equations and calculations may now be presented for solving any possible system of combustion. For this combustion problem liquid hydrogen and liquid oxygen will be burned. However, by simply rearranging some of the basic steps, any oxidizer - fuel combination, may be used.

Now before the reaction equations can be written, a decision must be made as to what products of combustion are likely to be present in the combustion gas. For the adiabatic reaction, the equilibrium flame temperature will be very high and a considerable amount of dissociation can be expected.

A basic knowledge of chemistry is required to determine the possible products. By comparing the equilibrium constants of the selected products, some may be eliminated by observing that their K_p value is several orders of magnitude less than the values listed for the other reactions. The presence of other combinations may be discounted when the experimental fact is considered that a chemical system will tend to adjust itself so that the constituents are in their lowest energy state. After a decision has been reached with regard to the products of combustion, the reaction equations can then be written.

In the combustion of liquid oxygen and liquid hydrogen, a possible assumption of probable products are, H_2 , O_2 , H_2O , O , H , OH , O_3 , and H_2O_2 . O_3 and H_2O_2 can be eliminated by applying the above-mentioned rules as these are both high energy forms.

The following equation



list the six assumed products of combustion. The value of $s/1$ will give the molar, oxidizer to fuel ratio. This can easily be converted to mass ratio, if desired, by use of the following equation

$$m = N M \quad (42)$$

However, for this problem only the molar ratio will be considered.

In the development of the system for solving for the molar values of the products of combustion it is necessary to regress a moment to discuss the selected system. "The errors are distributed among all the species" is the title of reference (2:142). This method is completely general and can be used irrespective of the number of substances present in the combustion products. The system is well suited for solution by electronic computers, which is the primary reason it was selected.

The system of equations used to determine the equilibrium composition at a given pressure and temperature is formed by linear equations representing the conservation of the species and by non-linear equations which can be written in logarithmic form and represent the various equilibria.

By referring to equation (41) and utilizing the basic equation for the balance of individual species

$$A_1 = \sum_1 n_1 \quad (43)$$

the first three equations may be formed.

1. Equation for hydrogen balance

$$2 = 2a + 2c + e + f \quad (44)$$

2. Equation for oxygen balance

$$2s = 2b + c + d + f \quad (45)$$

3. Equation for total moles

$$G = a + b + c + d + e + f \quad (46)$$

For any combustion problem, the number of products of combustion is equal to I, and the number of different species (atoms) is equal to J. Then from the equation

$$Y = I - J \quad (47)$$

the value of Y will determine the absolute number of independent equilibrium equations.

For this problem

$$Y = 6 - 2 \quad (48)$$

or

$$Y = 4 \quad (49)$$

Therefore, the number of independent equilibrium equations is 4. The basic equation for equilibrium in logarithmic form is

$$\log z_1 = \sum_{ij} a_j \log n_i \quad (50)$$

which allows the formation of the following four additional equations.

The values of K_p listed in NACA Report 1037 and also in the Appendix are based on the constituents being formed from their atoms. Therefore, the equations become

4. H₂O Equilibrium Equation, which is formed from



and results in

$$K_p(H_2O) = \frac{((c/G)P)}{((e/G)P)^2 (d/G)P} \quad (52)$$

which by rearranging becomes

$$K_p(H_2O) = \frac{c}{e^2 d} \frac{G^2}{P^2} \quad (53)$$

Then by equating

$$K_p(H_2O) = K_{p1} \quad (54)$$

In logarithmic form equation (53) may be stated as

$$2 \log P + \log K_{p1} = \log c - 2 \log e - \log d + 2 \log G \quad (55)$$

5. H₂ Equilibrium Equation, which is formed from



and results in

$$K_p(H_2) = \frac{(a/G)P}{((e/G)P)^2} \quad (57)$$

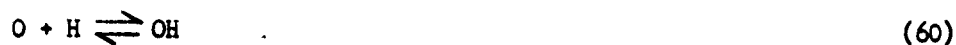
which by rearranging becomes

$$K_p(H_2) = \frac{a}{e^2} \frac{G}{P} \quad (58)$$

Then by defining $K_p(H_2)$ as K_{p2} and writing in logarithmic form, equation (58) may be stated as

$$\log P + \log K_{p2} = \log a - 2 \log e + \log G \quad (59)$$

6. OH Equilibrium Equation, which is formed from



and results in

$$K_p(OH) = \frac{(f/G)P}{(d/G)P (e/G)P} \quad (61)$$

which by rearranging becomes

$$K_p(OH) = \frac{f}{de} \frac{G}{P} \quad (62)$$

Then by defining $K_p(\text{OH})$ as K_{p3} and writing in logarithmic form, equation (61) may be stated as

$$\log P + \log K_{p3} = \log f - \log d - \log e + \log G \quad (63)$$

7. O_2 Equilibrium Equation, which is formed from



and results in

$$K_p(\text{O}_2) = \frac{(b/G) p}{((d/G)P)^2} \quad (65)$$

which by rearranging becomes

$$K_p(\text{O}_2) = \frac{b}{d^2} \frac{G}{P} \quad (66)$$

Then by defining $K_p(\text{O}_2)$ as K_{p4} and writing in logarithmic form, equation (65) may be stated as

$$\log P + \log K_{p4} = \log b - 2 \log d + \log G \quad (67)$$

This results in an array of mathematical logic consisting of seven equations and seven unknowns. Such a system can be solved by trial and error. It can be linearized by choosing arbitrary values for the number of moles (n_1^0) and then solving for an error function (X_1^0). The error functions are used in the following equation

$$n_1 = n_1^0 (1 + X_1^0) \quad (68)$$

If X_1^0 is sufficiently small, equation (68) in logarithmic form may be written as

$$\log n_1 \approx \log n_1^0 + X_1^0 \quad (69)$$

This is true by considering the fact that the $\log(1 + \text{small number})$ is approximately equal to the small number.

Equations (43), (44), (45), and (46) can thus be written in

the form

$$\sum_i a_i n_i^o x_i^o = A_1 - \sum_i a_i n_i^o = A_1 - A_1^o \quad (70)$$

where

$$A_1^o = \sum_i a_i n_i^o \quad (71)$$

Equations (55), (59), (63), and (67) can be written in the form

$$\sum_{ij} a_j x_i^o = \log z_1 - \sum_{ij} a_j \log n_i^o = \log \frac{z_1}{z_1^o} \quad (72)$$

where

$$\log z_1^o = - \sum_{ij} a_j \log n_i^o \quad (73)$$

The transformation of the variables is now complete. The new system is linear with respect to the error function (x_i) and can thus be solved by any standard method of solving simultaneous linear equations. The selected method is well suited for solution by electronic computers.

A complete description for the selected method to solve simultaneous linear equations is presented in the Appendix. The program is a partial replica of a method listed in the IBM listing of selected programs for the 1620 computer. (5.0.007) The original program was based on the original FORTRAN system and had to be completely rewritten so as to be suitable for use with the present FORTRAN program.

Table I, on the following page, consists of the seven linear equations of combustion consolidated into a matrix form. A detailed example is attached to Table I. It is available for additional reference, as required, to complete the formation of a similar system of equations necessary to solve other combustion problems.

TABLE I

COMBUSTION PROBLEM IN MATRIX FORM

	1. H_2 a	2. O_2 b	3. H_2O c	4. O d	5. H e	6. OH f	7. G g	$a^0 \quad b^0 \quad c^0 \quad d^0 \quad e^0 \quad f^0 \quad g^0$						
H														
1. Bal.	2a	XA	0	XB	2c	XC	0	XD	e	XE	f	XF	0	XG = 2 - (2a + 2c + f) = A1
O	0	XA	2b	XB	c	XC	d	XD	0	XE	f	XF	0	XG = 2S - (2b + c + d + f) = A2
2. Bal.														
N	a	XA	b	XB	c	XC	d	XD	e	XE	f	XF	-GH	XG = G - (a + b + c + d + e + f) = A3
3. Total														
4.	0	XA	0	XB	1	XC	-1	XD	-2	XE	0	XF	+2	XG = 2log p + Pk1 - (log c - 2log e - log d + 2log G) = A4
5.	1	XA	0	XB	0	XC	0	XD	-2	XE	0	XF	+1	XG = log p + Pk2 - (log a - 2log e + log G) = A5
6.	0	XA	0	XB	0	XC	-1	XD	-1	XE	1	XF	+1	XG = log p + Pk3 - (log f - log e - log d + log G) = A6
7.	0	XA	+1	XB	0	XC	-2	XD	0	XE	0	XF	+1	XG = log p + Pk4 - (log b - 2log d + log G) = A7

The following examples illustrate how the above matrix is set up:

$$A_1 = \sum_i a_i n_i \quad ** \quad n_i = n_i^0(1 + X_i) \quad ** \quad \sum_i a_i n_i^0 X_i^0 = A_1 - \sum_i a_i n_i^0$$

$$2 = 2a + 2c + e + f = 2a^0 + 2a^0 XA + 2c^0 + 2c^0 XC + e^0 + e^0 XE + f^0 + f^0 XF$$

$$2 = 2a^0 XF + f^0 XF = 2 - (2a^0 + 2c^0 + e^0 + f^0)$$

$$\log z_1 = \sum_{ij} a_j \log n_i \quad ** \quad \log n_i = \log n_i^0 + X_i \quad ** \quad \sum_{ij} a_j X_i = \log z_1 - \sum_{ij} a_j \log n_i^0$$

$$2 \log P + Pk1 = \log c - 2 \log e - \log d + 2 \log G$$

$$2 \log P + Pk1 = \log c^0 + XC - 2 \log e^0 - 2 XE - \log d^0 - XD + 2 \log G^0 + 2 XG$$

$$XC - 2 XE - XD + 2 XG = 2 \log P + Pk1 - (\log c^0 - 2 \log e^0 - \log d^0 + 2 \log G^0)$$

The value of X_1 obtained from the solution of the matrix provides the new value of n_1^1 which is computed, for the second approximation, from the equation

$$n_1^1 = n_1^0 (1 + X_1) \quad (74)$$

A very important consideration is that the first approximation may not be very close to the correct value. It is probable that during the first few trials a value for X_1 of less than -1.00 may be computed. The program will not accept a value for X_1 of -1.00 or less; a value greater than -1.00 must then be used. In this problem -0.995 was utilized for such cases with complete success. After the assumed values are within the correct range a value of less than -1.00 will never be calculated and the calculated values of X_1 may be used completely. At this time the computer may be set to compute continuously until the desired convergence is obtained.

When the calculated error functions have a value of equal to or less than -1.00 and are then used in equation (74), a negative or zero value is calculated for n_1 . This creates errors in the calculation resulting from the computer attempting to take the log of a negative or zero number. By inserting -0.995, a very small positive value of n_1 is calculated. This answer is approximately correct since it would be impossible to actually have a negative value of a constituent.

The initial selected values for the number of moles of the products of combustion are completely arbitrary; however, if any information on the approximate values is available, it should be utilized. After the problem is solved one time it is advisable to use the calculated values

as the original selected values for the number of moles in solving the problem for the new temperature selection as determined by Figure 4-1.

This will allow the problem to converge quicker and save having to replace the error functions that are equal to or less than -1.00.

Another suggestion is to require the sum of the first selected values not to exceed the value of the number of moles of the reactants.

The convergence of the system is given by the expression

$$\text{CONV} = /A_1 - A_1^0/ + /...../ + / \ln \frac{z_1}{z_0} / + /.....? \quad (75)$$

In the computer program, the value of $A_1 - A_1^0$ is set equal to A1 and the value of the $\log \frac{z_1}{z_0}$ is set equal to A4. By reference to the initial equations (44) and (55), it is quite apparent that when the correct values for the number of moles of the products have been computed A1, A2, A3, A4, A5, A6, and A7 will all be equal to zero.

When the computer does not have the ability to add absolute values, a simple method that may be used calls for adding the sum of $\sqrt{x \cdot x}$. The system is solved when the value of C becomes sufficiently small.

The method described above will now be applied in the solution of a problem involving the selected propellants of liquid oxygen and liquid hydrogen.

The Kp values listed in NACA 1037 are presented in logarithmic form to the base 10. The logarithmic program on the 1620 computer is based on the Napierian Logarithm Scale. To be consistent the values for Kp are multiplied by the natural logarithm of 10.

The computer program is subdivided into four parts:

1. Solution of the coefficients and the values for the solution column of the matrix.

2. Assignment of the appropriate values to columns and rows of the matrix program.
3. Solution of the matrix program.
4. Solution of the difference in enthalpies.

The value for the total number of moles has been assigned to G and GH in the computer program. The matrix coefficient (GH) in position (3, 7) of the developed matrix created some confusion, during the early stages of the problem. By experimentation it was found that by letting GH be equal to the new value for the total number of moles calculated from the value of XG and by letting the G equal the sum of the new values for the n_1 's the problem would converge. However, by reversing the value of G and GH the problem would not converge.

The computer program is designed to automatically replace any undesired error function with -0.995. This ability is dependent on the position of Sense Switch 3 which also controls the type out of solutions. When Sense Switch 3 is in the off position all values are typed out by the typewriter. During the type-out of the solution of the error functions, if one has a value of -1.00 or less, it is changed to -0.995. A message that this step has been completed is also typed out.

When the operator desires, Sense Switch 3 may be turned on to eliminate typing of all values except the value of convergence. This also eliminates the ability to change the error functions; therefore, it is important that the convergence value must be observed to be decreasing before this step is performed. If Sense Switch 3 is turned on prematurely and an undesired value of an error function is computed, an error statement will be typed out indicating that the computer has

been requested to take the logarithm of a negative number. The solution must be restarted as all values are then incorrect.

As the convergence approaches the desired limit, Sense Switch 3 may be turned off. This allows all values to be typed out which are then the correct solutions for the number of moles of each of the products of combustion.

By turning on Sense Switch 2, the computer branches to the fourth subdivision, where the difference in enthalpies is computed.

The computer also has been programed to interpolate linearly, as necessary, all values of input data. The value of RS is the fractional value between hundreds of degrees. If it is desired to compute for 3528 K, values for 3500 K and 3600 K are read into the computer. The value of RS is then 0.28.

The present computer, with 20,000 storage locations, did not have sufficient locations to compute the value of the molecular weight and the isentropic exponent. A second program was written to perform this computation. The last step of the first program is the command to punch out on data cards, the solution for the number of moles of each of the products. These solution cards are then used in the second program with the necessary additional data to compute the molecular weight and the isentropic exponent. This program also has the ability to interpolate linearly the necessary data.

For the design calculations in this problem the reactants will be assumed to be at standard conditions (298.16 K). The problem is then solved for a particular molar ratio and a selected chamber or total pressure (23 atmospheres). The necessary values are taken from

NACA 1037 by assuming a particular combustion temperature. The combustion products and the change in enthalpies (ΔH) are then calculated. ΔH is defined as the enthalpy of the products taken at the combustion temperature minus the enthalpy of the reactants taken at the temperature prior to combustion. If the assumption for the combustion temperature is correct, ΔH will be equal to zero. If $\Delta H > 0$ the assumed temperature was too high; a lower value must be chosen, and combustion of the gas must be recalculated for the new temperature. Of course, if $\Delta H < 0$ then a larger value for the temperature must be selected. Repetition of this procedure two or three times will usually yield the correct value of temperature, by graphical interpolation.

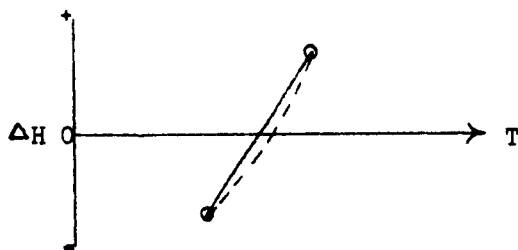


Figure 4-1. Interpolation for adiabatic flame temperature.

If the first two assumed values of temperature give values of ΔH on each side of the zero line as shown in Figure 4-1, an approximate value of the combustion temperature may be determined by linear interpolation; however, since the curve of ΔH vs T is usually concaved up, the value so determined will usually be less than the actual temperature.

Linear interpolation for the proper values of H and K_p is acceptable. It should be noted that linear interpolation for K_p over a wide temperature ranges is not accurate, and logarithmic interpolation is required for adequate approximations. However, the equilibrium constants in

NACA 1037 are tabulated for every one hundred degrees Kelvin and linear interpolation within this range of temperature yields sufficiently accurate results.

The following pages consisting of Table II and Table III have the complete computer program for liquid hydrogen and liquid oxygen. With the previous explanations and a basic knowledge of the IBM 1620 FORTRAN system, no problem should exist in setting up the program to compute the combustion properties for any propellant combination.

TABLE II
FIRST COMPUTER PROGRAM

```

      DIMENSION X(7,8)
81  FORMAT(//(F12.8))
32  FORMAT(//8HSOLUTION)
33  FORMAT(44HDIAGONAL THAT IS LESS THAN OR EQUAL TO TOLER)
34  FORMAT(2HIS I3)
40  FORMAT(E11.8)
      READ40, PK1,PK2,PK3,PK4,PS,S,TOLER,RS
      READ40,PK1A,PK2A,PK3A,PK4A
      READ40,A,B,C,D,E,F
      READ 40,XA,XB,XC,XD,XE,XF,XG
      PK1=PK1 - RS*(PK1 - PK1A)
      PK2=PK2 - RS*(PK2 - PK2A)
      PK3=PK3 - RS*(PK3 - PK3A)
      PK4=PK4 - RS*(PK4 - PK4A)
27  G=A+B+C+D+E+F
      A=A*(1.+XA)
      B=B*(1.+XB)
      C=C*(1.+XC)
      D=D*(1.+XD)
      E=E*(1.+XE)
      F=F*(1.+XF)
      GH=G*(1.+XG)
      G=A+B+C+D+E+F
      H=LOG(10.)
      A1=2.-(2.*A+2.*C+E+F)
      A2=2.*S-(2.*B+C+D+F)
      A3 = G-(A+B+C+D+E+F)
      A4=2.*(LOG(PS))+H*PK1-(LOG(C)-2.*LOG(E)-LOG(D)+2.*LOG(G))
      A5=(LOG(PS))+H*PK2-(LOG(A)-2.*LOG(E)+LOG(G))
      A6=(LOG(PS))+H*PK3-(LOG(F)-LOG(E)-LOG(D)+LOG(G))
      A7=(LOG(PS))+H*PK4-(LOG(B)-2.*LOG(D)+LOG(G))
      CONV=SQRT(A1*A1)+SQRT(A2*A2)+SQRT(A3*A3)+SQRT(A4*A4)+SQRT(A5*A5)
      CONV=CONV+SQRT(A6*A6)+SQRT(A7*A7)
      IF (SENSE SWITCH 3)50,51
51  PRINT81,A1,A2,A3,A4,A5,A6,A7
      PRINT 81,A,B,C,D,E,F,G,GH
50  PRINT 81,CONV
      IF(SENSE SWITCH 2)30,31
31  X(1,1)=2.*A
      X(2,1)=0.
      X(3,1)=A
      X(4,1)=0.
      X(5,1)=1.
      X(6,1)=0.
      X(7,1)=0.
      X(1,2)=0.

```

```

X(2,2)=2.*B
X(3,2)=B
X(4,2)=0.
X(5,2)=0.
X(6,2)=0.
X(7,2)=1.
X(1,3)=2.*C
X(2,3)=C
X(3,3)=C
X(4,3)=1.
X(5,3)=0.
X(6,3)=0.
X(7,3)=0.
X(1,4)=0.
X(2,4)=D
X(3,4)=D
X(4,4)=-1.
X(5,4)=0.
X(6,4)=-1.
X(7,4)=-2.
X(1,5)=E
X(2,5)=0.
X(3,5)=E
X(4,5)=-2.
X(5,5)=-2.
X(6,5)=-1.
X(7,5)=0.
X(1,6)=F
X(2,6)=F
X(3,6)=F
X(4,6)=0.
X(5,6)=0.
X(6,6)=1.
X(7,6)=0.
X(1,7)=0.
X(2,7)=0.
X(3,7)=-GH
X(4,7)=2.
X(5,7)=1.
X(6,7)=1.
X(7,7)=1.
X(1,8)=A1
X(2,8)=A2
X(3,8)=A3
X(4,8)=A4
X(5,8)=A5
X(6,8)=A6
X(7,8)=A7
N = 7
N1 = N + 1
DO 14 I = 1, N, 1

```

```

      DIAG = X(I,I)
      IF (DIAG) 3, 20, 4
3 IF (DIAG + TOLER) 5, 19, 19
4 IF (DIAG - TOLER) 19, 19, 5
5 DO 6 J = 1, N1
6 X(I,J) = X(I,J) / DIAG
  K = 1
  9 IF (K-I) 11, 13, 11
11 FELMT = X(K,I)
  DO 12 J = 1, N1
12 X(K,J) = X(K,J) - FELMT * X(I,J)
13 K = K + 1
  IF (K-N) 9, 9, 14
14 CONTINUE
  IF (SENSE SWITCH 3) 1, 28
28 J = N1
  TYPE 32
  DO 18 I=1, N
  TYPE 40, X(I,J)
  IF (X(I,J) + 1.0) 65, 65, 18
65 X(I,J) = -.995
  TYPE 66
66 FORMAT(41H THE ABOVE VALUE HAS BEEN CHANGED TO -.995)
18 CONTINUE
  GO TO 1
19 TYPE 33
  TYPE 34, I
  GO TO 5
20 STOP
  1 XA=X(1,8)
  XB=X(2,8)
  XC=X(3,8)
  XD=X(4,8)
  XE=X(5,8)
  XF=X(6,8)
  XG=X(7,8)
  GO TO 27
30 READ 40, H2S, O2S, H2, O2, H2O, O, H, OH
  READ 40, H2A, O2A, H2OA, OA, HA, OHA
  OH = OH + RS*(OHA - OH)
  H = H + RS*(HA - H)
  O = O + RS*(OA - O)
  H2O = H2O + RS*(H2OA - H2O)
  O2 = O2 + RS*(O2A - O2)
  H2 = H2 + RS*(H2A - H2)
  HTS=H2S+S*O2S
  HTC=A*H2 + B*O2 + C*H2O + D*O + E*H + F*OH
  DELH=HTC-HTS
  PRINT 41, HTC, HTS, DELH
41 FORMAT (//(E14.8))
  PUNCH 40, A, B, C, D, E, F
  STOP
  END

```


TABLE III

SECOND COMPUTER PROGRAM

```

67 FORMAT (//(35HTHE MOLECULAR WEIGHT OF THE MIX IS F10.5))
68 FORMAT(28HTHE CP VALUE FOR THE MIX IS F10.5)
69 FORMAT (23HTHE VALUE FOR CP/CV IS F10.5)
40 FORMAT(E11.8)
  READ 40,A,B,C,D,E,F,S,RS
  READ 40, CH2, CO2, CH2O, CO, CH, COH
  READ 40, CH2A, CO2A, CH2OA, COA, CHA, COHA
  G=A+B+C+D+E+F
  CH2 = CH2 + RS*(CH2A - CH2)
  CO2 = CO2 + RS*(CO2A - CO2)
  CH2O = CH2O + RS*(CH2OA - CH2O)
  CO = CO + RS*(COA - CO)
  CH = CH + RS*(CHA - CH)
  COH = COH + RS*(COHA - COH)
  CPM = CH2*A/G + CO2*B/G + CH2O*C/G + CO*D/G + CH*E/G + COH*F/G
  CVM = CPM - 1.98718
  CK = CPM/CVM
  CMOL = 2.*A/G + 32.*B/G + 18.*C/G + 16.*D/G + 1.*E/G + 17.*F/G
  PRINT 67,CMOL
  PRINT 68,CPM
  PRINT 69,CK
  STOP
  END

```

CHAPTER V

RESULTS OF CALCULATIONS

The results based on a combustion pressure of 23 atmospheres are the primary concern of this report. A graph relating the flame temperature, isentropic exponent, and molecular weight of the products, to the oxidizer-fuel ratio, is presented in Figure 5-2. In addition a very interesting theory of rocketry is proven - the temperature of the gases depends primarily on the oxidizer-fuel ratio, and to a small extent on combustion pressure. The latter depends, of course, on the rate at which the propellants are being consumed and the throat area of the exhaust nozzle. The curve of the flame temperatures based on a combustion pressure of 20 atmospheres is presented for demonstration of the effect resulting from varying the combustion pressure.

The program is set up for the IBM 1620 computer as described in Chapter IV. To facilitate the calculations of the initial constants and coefficients for the matrix program, the value of zero must be read in for the error functions XA, XB, XC, XD, XE, XF, and XG. A temperature is selected for which the equilibrium constants are taken from NACA 1037. In addition to the four Kp constants, values for the molar ratio (S), combustion pressure (PS), tolerance level (TOLER), and a value for the fractional number of degrees (RS) have to be read in to the computer. The tolerance level and its use are explained in the Appendix.

Subdivision three of the first computer program, consisting of the solution of the seven linear equations, has almost entirely been taken from the program listed in the Appendix. The input section has been

deleted, since each individual position of the matrix has been identified in subdivision two. The portion evaluating a zero diagonal has been amended because the only way to adjust the rows or columns of the matrix is to rewrite the program. Care should be taken in the original writing of the computer program to prevent a zero major diagonal. Specific instructions are given in the Appendix.

A tolerance level value of 0.00001 was read in at the beginning of the program. The section permitting changing of the tolerance level was omitted from the computer program. The tolerance level in this program is not very important since the calculated values of the error functions are only used to create new assumed selections for the products of combustion. As long as the convergence continues to decrease the program is successful.

The computer program has been written to interpolate, when necessary, the input data for a selected temperature falling between hundreds of degrees. An example may be illustrated by assuming the desired temperature is 3528 K. A value for RS of 0.28 must be entered in the computer along with the appropriate input data selected at 3600 K and 3500 K. The data consisting of the four Kp constants, and the enthalpy of the constituents are taken from the NACA 1037 tables in the Appendix.

The values listed in Table IV are computed from an oxidizer/fuel molar ratio of 0.5 and with a combustion pressure of 23 atmospheres. The computation was completed for temperatures of 3400 K, 3500 K, and 3600 K. The calculated values of the moles of the products are given in Table II along with the value of ΔH computed for each of the three temperatures. These values of ΔH are plotted on the graph in Figure 5-1, and then

graphically interpolated for the temperature for which ΔH is zero. The temperature was determined to be 3528 K. The problem was then computed again for a temperature of 3528 K and the resulting ΔH was within the required accuracy. As proof, the problem was then computed at 3525 K to get an estimate of the change of ΔH per degree Kelvin. The ΔH at 3528 K was +0.06076 while the ΔH at 3525 K was -0.10568. This was sufficient proof that the temperature of 3528 K was within the experimental accuracy possible in the combustion chamber of a rocket engine.

TABLE IV
RESULTS OF CALCULATIONS
FOR O/F RATIO OF (0.5) AND 23 ATMOSPHERES

Temp. K	3400	3500	3525	3528	3600
H ₂	0.1325	0.1545	0.1602	0.1609	0.1779
O ₂	.0429	.0491	.0506	.0508	.0554
H ₂ O	.8015	.7629	.7527	.7515	.7199
O	.0183	.0257	.0279	.0281	.0354
H	.0375	.0518	.0560	.0565	.0704
OH	<u>.0944</u>	<u>.1132</u>	<u>.1182</u>	<u>.1188</u>	<u>.1338</u>
G	1.1271	1.1572	1.1656	1.1666	1.1928
ΔH	-6.5760	-1.4671	-0.1057	+0.0608	+4.2998

Since the second computer program was also written to compute a linear interpolation for necessary input data, it is only required to read into the computer C_p values for the six products of combustion at temperatures of 3600 K and 3500 K. In addition, as stated before, the

computed values taken from the first program for the number of moles, the value of S, and the value of RS have to be entered as input data into the computer. The particular values of molecular weight were permanently written into the program.

The value for the molecular weight of the mixture is computed from the following equation

$$M = (a/G)M_{H_2} + (b/G)M_{O_2} + (c/G)M_{H_2O} + (d/G)M_O + (e/G)M_H + (f/G)M_{OH} \quad (76)$$

This value, for an O/F ratio of 0.5 and a combustion pressure of 23 atmospheres, was computed as

$$M = 15.42976 \quad (77)$$

The value for Cp of the mixture is computed from the following equation

$$Cp_{mixture} = (a/G)Cp_{H_2} + (b/G)Cp_{O_2} + (c/G)Cp_{H_2O} + (d/G)Cp_O + (e/G)Cp_H + (f/G)Cp_{OH} \quad (78)$$

This value was determined to be

$$Cp_{mixture} = 11.44081 \frac{\text{Cal}}{\text{gmole-K}} \quad (79)$$

From the thermodynamic identity which relates the specific heat at constant volume (Cv) to that at constant pressure (Cp), Cv will now be computed from the equation

$$Cv = Cp - Ru \quad (80)$$

where

$$Ru = 1.98718 \frac{\text{Cal}}{\text{gmole-K}} \quad (81)$$

Then from equation (79) and (80)

$$Cv = 11.44081 - 1.98718 \quad (82)$$

or

$$C_v = 9.45363 \frac{\text{Cal}}{\text{gmole-K}} \quad (83)$$

The isentropic exponent (k) is the ratio of the specific heats and is

$$k = \frac{C_p}{C_v} \quad (84)$$

or

$$k = \frac{11.44081}{9.45363} \quad (85)$$

then

$$k = 1.21020 \quad (86)$$

Table V consists of tabulated values from the calculations at different O/F ratio while holding the combustion pressure constant at 23 atmospheres. These values were computed with the same procedures as have been illustrated for an O/F ratio of 0.5

The tabulated results of the change in adiabatic flame temperature, caused by changing the combustion pressure to 20 atmospheres, is presented in Table VI. Only the variation of the flame temperature is available in Table VI as this is the only variation of importance.

TABLE V
FINAL RESULTS OF CALCULATIONS
COMBUSTION PRESSURE 23 ATMOSPHERES

O/F Molar Ratio		0.2	0.3	0.4	0.5	0.6	0.7
Moles in Products	Tc K	<u>2777</u>	<u>3300</u>	<u>3492</u>	<u>3528</u>	<u>3495</u>	<u>3440</u>
	H ₂	0.5950	0.3942	0.2476	0.1609	0.1099	0.0788
	O ₂	.0000	.0013	.0139	.0508	.1106	.1865
	H ₂ O	.3979	.5679	.6830	.7515	.7961	.8270
	O	.0001	.0023	.0131	.0281	.0395	.0460
	H	.0121	.0486	.0627	.0565	.0448	.0345
	OH	<u>.0020</u>	<u>.0272</u>	<u>.0761</u>	<u>.1188</u>	<u>.1432</u>	<u>.1541</u>
	G	1.0071	1.0415	1.0964	1.1666	1.2441	1.3269
	M	8.3405	11.1377	13.4985	15.4298	17.0399	18.3909
Cal g-mole-K	Cp	10.2839	11.0239	11.3384	11.4408	11.4600	11.4360
	Cv	8.2967	9.0367	9.3512	9.4536	9.4728	9.4488
	k	1.2395	1.2199	1.2125	1.2102	1.2098	1.2103

TABLE VI
FINAL RESULTS OF CALCULATIONS
COMBUSTION PRESSURE 20 ATMOSPHERES

O/F Molar Ratio		0.2	0.3	0.4	0.5	0.6	0.7
Tc K		2758	3280	3470	3505	3476	3411

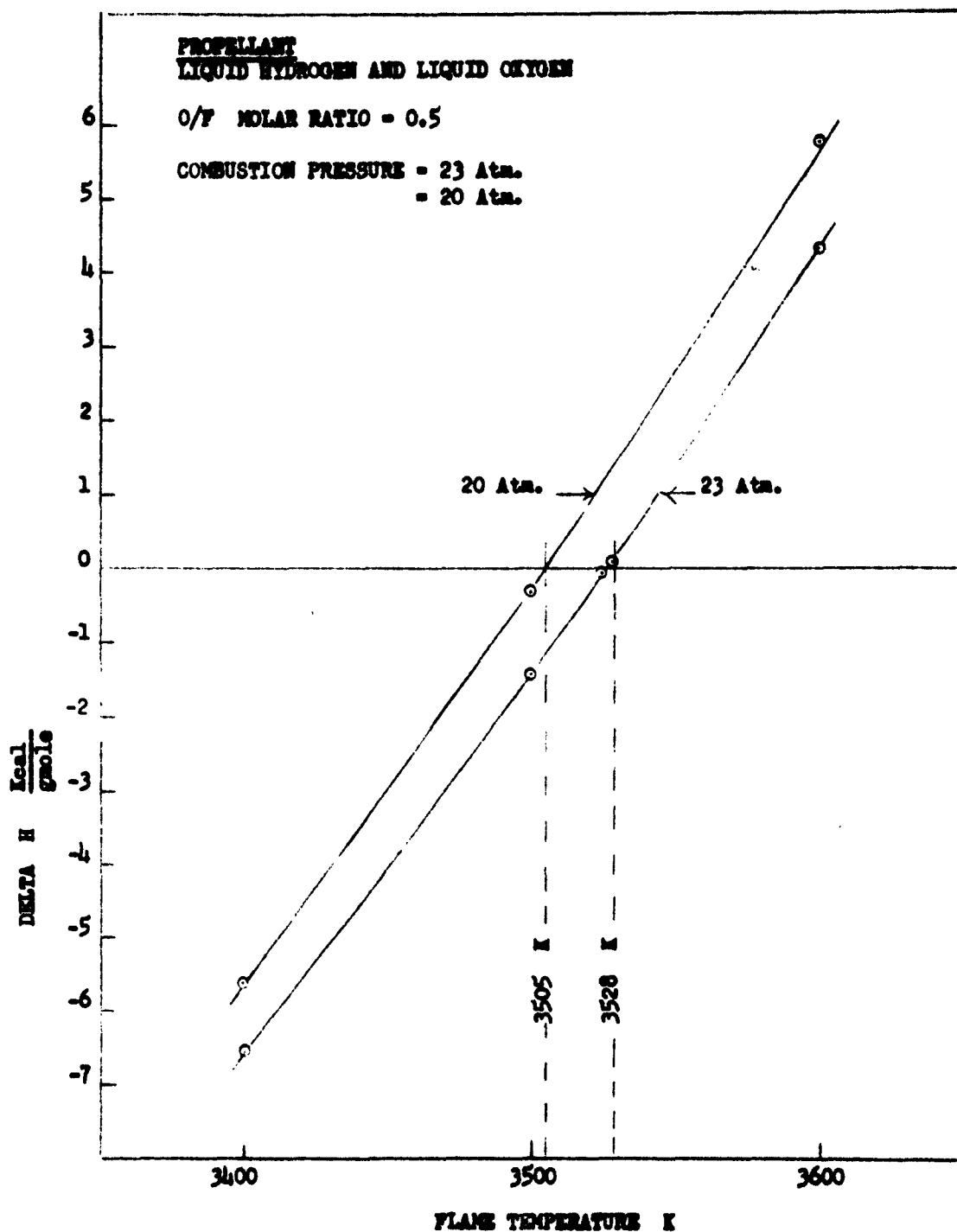


Figure 5-1. Graphical Interpolation for Combustion Flame Temperature

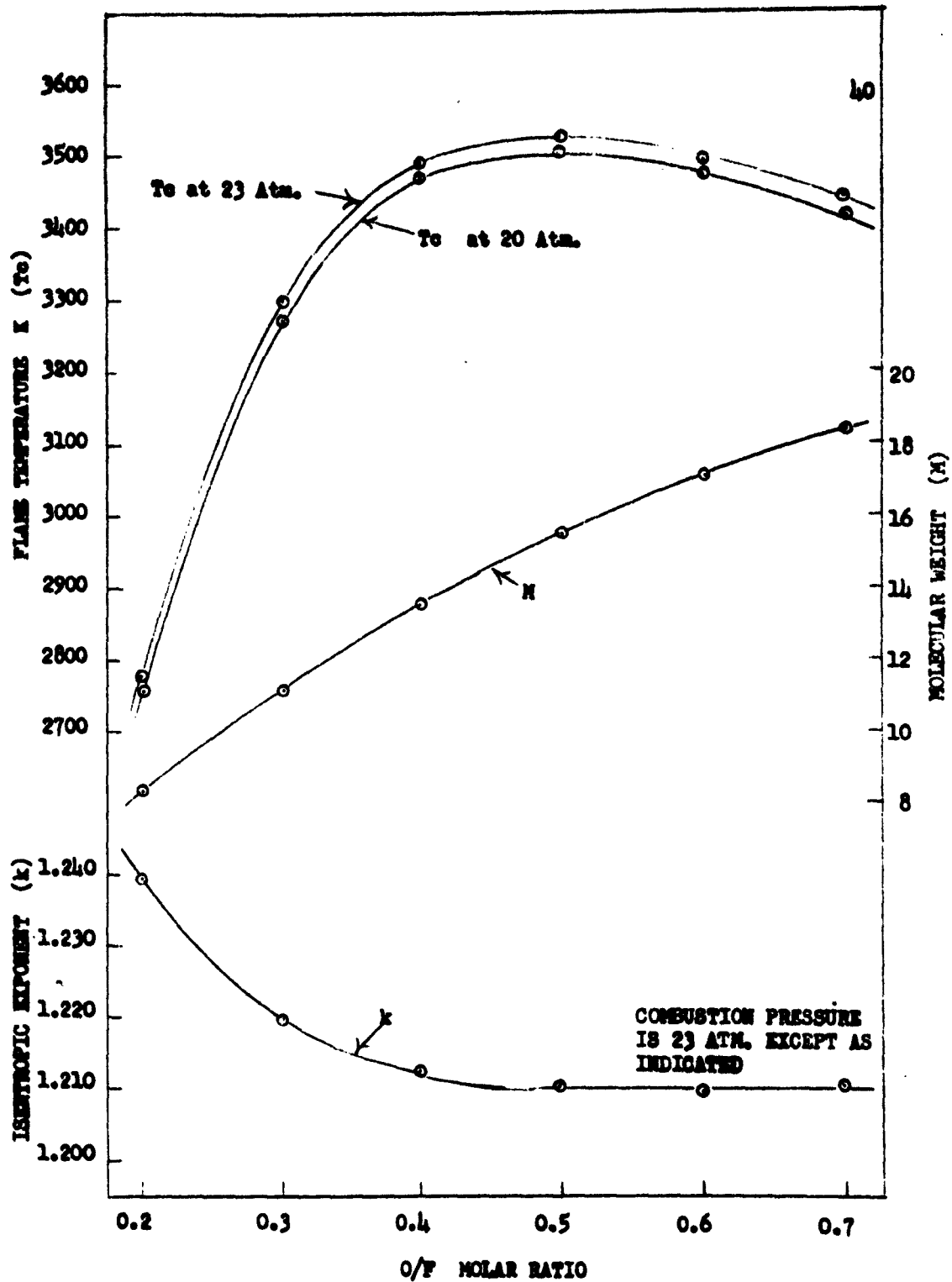


Figure 5-2. Graphical Results For Liquid Hydrogen and Liquid Oxygen

TABLE VII
RESULTS FROM FIRST PROGRAM

-.30000000 A1
-.10000000 A2
.00000000 A3
4.48435890 A4
2.05136710 A5
1.34662590 A6
1.48234660 A7

The following four pages are the
computer results from the following
input data:

.40000000 H₂
.10000000 O₂
.40000000 H₂O
.10000000 O
.30000000 H
.40000000 OH
1.70000000 G
1.70000000 GH

Initial assumption
for products of
combustion.

T	3528 K
O/F	0.5
TOLER	0.00001
PS	23 Atmospheres

9.76469830

Initial convergence value

SOLUTION

-.52371340E-00 XA
-.43600000E-00 XB
.11604744E+01 XC
-.11695445E+01 XD
THE ABOVE VALUE HAS BEEN CHANGED TO -.995
-.14979106E+01 XE
THE ABOVE VALUE HAS BEEN CHANGED TO -.995
-.90008880E-00 XF
-.42074042E-00 XG

Results of initial calculations

for the error functions.

-.15087310
-.01745420
.00000000
-11.40451800
-7.41533000
-6.55833300
-8.15338600

.19051464
.05640000
.86418976
.00050000
.00150000
.03996448
1.15306880
.98474132

33.69989100

SOLUTION

-.18793932E-00
.18042300E-02
-.75171440E-01
.40532358E+01
.35893352E+01
.11329576E+01
-.48720557E-01

-.00000020
-.00000000
.00000000
-6.57387400
-4.11718150
-4.12958100
-4.87263250

.15470945
.05650175
.79922741
.00252661
.00688400
.08524254
1.10509170
1.09689070

19.69326700

SOLUTION

.34152510E-01
-.73875990E-01
-.34020070E-01
.24102371E+01
.20865257E+01
.34546440E-00
.21717281E-01

-.00000010
-.00000010
.00000000
-3.10104200
-1.91799860
-2.09381940
-2.36364870

.15999316
.05232763
.77203769
.00861636
.02124765

.111469080
1.12891320
1.12909120

9.47650880

3.06712780

Here Sense Switch 3 was turned on.

.44407657

.01147719

.00000870

Here Sense Switch 3 was turned off.

SOLUTION

.38571400E-06
-.58173300E-06
.43619820E-07
.15603613E-05
.49408466E-06
-.14800950E-06
.10245536E-06

The values of the error
functions are now very small
numbers.

.00000010 A1
-.00000000 A2
.00000000 A3
-.00000020 A4
-.00000010 A5
-.00000020 A6
-.00000020 A7

.16086923 H₂
.05080107 O₂
.75149282 H₂O
.02813721 O
.05650815 H
.11876787 OH
1.16657620 G
1.16657620 GH

Final values for the
products of combustion.

.00000080

Final convergence value

.71556908E+02
.71496150E+02
.60758000E-01

Enthalpy of products at 3528 K
Enthalpy of reactants at 298.16 K
 ΔH

STOP

TABLE VIII

RESULTS FROM SECOND PROGRAM

THE MOLECULAR WEIGHT OF THE MIX IS 15.42976
THE CP VALUE FOR THE MIX IS 11.44081
THE VALUE FOR CP/CV IS 1.21020
STOP

BIBLIOGRAPHY

BIBLIOGRAPHY

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APPENDIX

SOLUTION OF SIMULTANEOUS LINEAR EQUATIONS

Introduction

This program is a replica of program number (5.0.007) from the IBM 1620 General Program Library. It has been rewritten as necessary to be compatible with the present 1620 (20K) computer and the FORTRAN programming system with format statements. Although this program was tested by its author using the sample problems, no warranty, expressed or implied, is made by the author or IBM.

Description of the Program

A knowledge of the IBM 1620 FORTRAN system is required to understand the following program.

This program solves sets of non-homogeneous simultaneous linear equations and provides either typewriter or punched card output. Up to 25 equations in 25 unknowns may be solved. The first card read for each set of equations states the number of equations following. The program automatically sizes itself for the proper matrix dimensions. Any number of sets of equations may be solved one after the other without reloading the program deck. When a solution has been obtained the word SOLUTION is typed. Under this heading the solution variables are typed one per line in the order in which they appear from left to right in the original equations. Punched card output is identical, with one card punched for each line typed.

If a set of equations is submitted which has more than one solution, a valid solution will be typed or punched, but no indication will be given that there are other solutions as well.

If the equations in the set are not all independent, a typewriter message will indicate that a diagonal element is zero. No solution is developed in this case, as there are infinite solutions to the set of equations.

Additional information regarding the characteristics of the program is contained in the discussion of the method of computation.

Method of Computation

General Description. The Jordan method of elimination¹ is used to accomplish the solution. Briefly this method consists of diagonalizing the augmented coefficient matrix. After diagonalization the right hand or augmented column contains the solution values for the variables.

The reduction of the matrix takes place in the same storage locations where the original coefficients are stored. Thus at the completion of the solution the original coefficients are lost, and in

¹ Alston S. Householder, Principles of Numerical Analysis (New York: McGraw-Hill Book Co., Inc., 1953), pp. 68-72.

their place remain an identity matrix and the column of answers.

Division by a Zero Diagonal. In the process of diagonalization the elements of each row to the right of the diagonal and the diagonal itself are divided by the diagonal element. The diagonal elements are used in the same order in which they appear in the original matrix. No attempt is made to select these pivotal elements by magnitude. Hence a zero must not appear on the diagonal of the matrix. If such a condition exists, a message will be typed indicating which diagonal element is zero and control passes to reading the next problem.

The possibility of zero diagonal elements may be minimized by observing two rules in laying out the original matrix.

1. The upper left hand element should not be zero.
2. No diagonal element may be zero if all elements in the row to the left of it are zero.

There is a slight chance of generating a zero diagonal element in the course of calculations. Equations which are not independent (a unique solution undefined) will also generate a zero diagonal. If it is known that the coefficient matrix is non-singular, that is, that there is a unique solution, division by zero may be easily corrected and the problem submitted again. A simple rearrangement of the columns will usually suffice. In rearranging the columns the equality vector always must be kept on the right. As indicated later, rearrangement of columns may be accomplished simply by rearranging input cards. No additional punching is required.

Tolerance warning Level. When the diagonal element is very small relative to the values to its right in the row, a loss of accuracy will result from round-off errors. In this program the operator has control over this situation. When the absolute value of the divisor is less than or equal to some tolerance level selected by the operator, a warning message is typed. The operator then has the choice of continuing with the solution or proceeding to the next problem. If he should elect to continue, he does so with the knowledge that the answer may contain significant rounding errors. Of course, checking the answers will quickly show the accuracy of the solution.

Input Card Format

The first card of the input for each set of equations must be a card with the number of equations punched according to the FORMAT STATEMENT (I2).

The matrix of coefficients is punched column-wise beginning with the left-most column and ending with the equality column. Each column must begin with a new card. A card must contain five values punched successively according to the FORMAT STATEMENT (E14.8). It is obvious

that the five values will take up the first 70 spaces on the card. The column may be continued over as many cards as necessary. (Five cards is the maximum number, as the program is limited to 25 unknowns.) If the number of rows is not a multiple of five, dummy zero values must be punched to finish out five entries on the last card of the column. It is never necessary to punch more than four dummy zero entries for a given column. The number of cards per column will be the same for all columns within a given problem, but may vary from problem to problem. The dummy entries used to fill out the five entries on the last card of a column need not be zero. These entries are accessed during the read in, but are never accessed during calculation. Hence they must be present, but their value is immaterial.

Output Card and Typewriter Format

The first statement for each problem will be the word SOLUTION followed by the answers typed according to FORMAT STATEMENT (E14.8). If it is desired to have the answers punched with the same format statement, Sense Switch 1 should be turned on. The word SOLUTION will not be punched; however, the answers including the word SOLUTION will continue to be typed. The cards will contain the solution, one per card in the order in which the variables appeared in the original matrix.

Sense Switch Settings

Sense Switch

1	ON	Solution is typed and punched.
	OFF	Solution is typed.
2	ON	Next problem after tolerance stop.
	OFF	Continue after tolerance stop.
3	ON	Tolerance level entered for each problem.
	OFF	Tolerance level entered only once.
4	ON	To correct error in typing tolerance level.
	OFF	Tolerance level entered correctly.

Normal Loading Procedure

1. Clear Storage
2. Depress RESET
3. Depress LOAD button
4. Depress READER START when hopper is empty
5. LOAD DATA is typed by typewriter
6. Enter data cards
7. Depress COMPUTER START
8. Depress READER START

Special Loading Instructions

At any time the program may be initialized and started by branching to 08300.

Other Instructions and Remarks

Tolerance Level. When the program begins, the typewriter will request the operator to enter the tolerance level as a floating point number in the form (+.000000).

If the entry is typed correctly, set Sense Switch 4 OFF, press RELEASE and COMPUTER START. The data cards will then be read.

If the entry is typed incorrectly, turn Sense Switch 4 ON, press RELEASE and START. The program will immediately return control to the typewriter so the entry may be made again. If the retry is correct, follow the procedure for a correct entry.

If it is desired to enter a tolerance level for each set of equations, turn Sense Switch 3 ON. If not, turn Switch 3 OFF, and the last tolerance level entered will automatically be applied to all succeeding sets of equations.

When a tolerance warning stop occurs, directions for the use of Switch 2 are typed. Only at this time is the setting of Switch 2 interrogated.

All programed stops are accompanied by typewriter messages which are self explanatory and which indicate the required action.

SAMPLE PROBLEMS

The following four problems were used one after the other.

$$8x_1 - 5x_2 + 7x_3 = 29$$

$$+2x_2 - 2x_3 = -2$$

$$-x_1 + 9x_2 - 6x_3 = 1$$

$$\text{Answer: } x_1 = 2, \quad x_2 = 3, \quad x_3 = 4$$

$$x_1 + 2x_2 + 3x_3 - 4x_4 + 5x_5 - 6x_6 + 7x_7 - 8x_8 = -28$$

$$7x_2 - 2x_5 + x_7 + x_8 = 19$$

$$2x_1 + 3x_2 - 4x_3 - 5x_4 + 6x_6 = 12$$

$$x_1 + x_2 + x_3 + x_4 + x_5 + x_6 + x_7 + x_8 = 36$$

$$10x_1 + 3x_2 - 4x_3 + x_5 + 2x_6 - 9x_7 = -42$$

$$3x_1 - 3x_2 - 2x_3 + 2x_4 + x_6 = 5$$

$$-8x_1 - 9x_3 + 7x_5 + 6x_7 - 3x_8 = 18$$

$$+3x_7 - 5x_8 = -19$$

$$\text{Answers: } x_1 = 1, \quad x_2 = 2, \quad x_3 = 3, \quad x_4 = 4$$

$$x_5 = 5, \quad x_6 = 6, \quad x_7 = 7, \quad x_8 = 8$$

$$3x_1 + 8x_2 + 6x_3 + 10x_4 + 42x_5 = -20$$

$$+2x_2 + x_4 + 5x_5 = 40$$

$$+ 4x_4 + 6x_5 = -18$$

$$2x_1 + 4x_2 + 7x_3 + 9x_5 = 12$$

$$x_1 + 4x_2 + 6x_3 - 2x_4 + 10x_5 = 7$$

This problem will cause diagonal 3 to be zero. It was included merely to illustrate the typewriter message.

$$\begin{aligned}
 3x_1 + 8x_2 + 6x_3 + 10x_4 + 42x_5 &= -20 \\
 +2x_2 &+ x_4 + 5x_5 = 40 \\
 &+ .01x_3 + 4x_4 + 6x_5 = -18 \\
 2x_1 + 4x_2 + 7x_3 &+ 9x_5 = 12 \\
 x_1 + 4x_2 + 6x_3 - 2x_4 + 10x_5 &= 7
 \end{aligned}$$

This problem will make diagonal 3 go below a tolerance level of 0.1. It was included merely to illustrate this typewriter message.

COMMENTS ON THE TYPEWRITER LOG FOR SAMPLE PROBLEMS

On the typewriter log, which follows, several points should be noted. Sense Switch 3 was on at the beginning. Note that a tolerance level was entered for each of the first three problems. After the tolerance was entered for the third problem, Sense Switch 3 was turned off. When diagonal 3 went to zero and COMPUTER START was pressed to continue with the fourth problem, the solution began immediately without the entry of a tolerance level, as Switch 3 was off. Note the tolerance level in the warning message of the fourth problem is the last entry made--that for problem 3. When this warning message appeared, Switch 2 was turned off and calculation continued to obtain a solution.

4908300RS
ACCEPT TOLERANCE IN FORM +.000000 PUSH RS
+.000001RS

SOLUTION
.20000000E+01
.30000000E+01
.40000000E+01
ACCEPT TOLERANCE IN FORM +.000000 PUSH RS
+.000001RS

SOLUTION
.10000065E+01
.19999976E+01
.30000053E+01
.39999963E+01
.49999916E+01
.59999990E+01
.70000022E+01
.80000012E+01
ACCEPT TOLERANCE IN FORM +.000000 PUSH RS
+.1RS
DIAGONAL IS ZERO, PUSH START FOR NEXT PROBLEM
IS 3

DIAGONAL THAT IS LESS THAN OR EQUAL TO TOLER
IS 3
TURN SW 2 OFF TO CONT. ON FOR NEXT PROBLEM
THEN PUSH START

SOLUTION
-.67605150E+01
.34405115E+02
-.70773320E+01
.59439480E+01
-.69508359E+01

SOURCE PROGRAM FOR SOLUTION OF SIMULTANEOUS LINEAR EQUATIONS

ENTER SOURCE PROGRAM
THEN PUSH START

```

      DIMENSION X(26,27)
30  FORMAT(12)
31  FORMAT(E11.8,E11.8,E11.8,E11.8,E11.8)
32  FORMAT(//8HSOLUTION)
33  FORMAT(14HDIAGONAL THAT IS LESS THAN OR EQUAL TO TOLER)
34  FORMAT(2HIS I3)
35  FORMAT(12HTURN SW 2 OFF TO CONT, ON FOR NEXT PROBLEM)
36  FORMAT(15HTHEN PUSH START)
37  FORMAT(15HDIAGONAL IS ZERO, PUSH START FOR NEXT PROBLEM)
38  FORMAT(14HACCEPT TOLERANCE IN FORM +.000000 PUSH RS)
39  FORMAT(F8.6)
40  FORMAT(E11.8)
10  PRINT 38
      ACCEPT 39, TOLER
1  READ 30, N
      N1 = N + 1
      DO 2 J = 1, N1
      DO 2 I = 1, N, 5
2  READ31,X(I,J), X(I+1,J), X(I+2,J), X(I+3,J), X(I+4,J)
      DO 14 I = 1, N, 1
      DIAG = X(I,I)
      IF (DIAG) 3, 20, 4
3  IF (DIAG + TOLER) 5, 19, 19
4  IF (DIAG - TOLER) 19, 19, 5
5  DO 6 J = I, N1
6  X(I,J) = X(I,J) / DIAG
      K = 1
9  IF (K-I) 11, 13, 11
11 FELMT = X(K,I)
      DO 12 J = I, N1
12 X(K,J) = X(K,J) - FELMT * X(I,J)
13 K = K + 1
      IF (K-N) 9, 9, 14
14 CONTINUE
      J=N1
      IF (SENSE SWITCH 1) 15, 17
15 TYPE 32
      DO 16 I = 1, N
      PUNCH 40, X(I,J)
16 TYPE 40, X(I,J)
      GO TO 21
17 TYPE 32
      DO 18 I=1 , N

```



```
18 TYPE 40, X(I,J)
21 IF (SENSE SWITCH 3) 10,1
19 TYPE 33
    TYPE 34,I
    TYPE 35
    TYPE 36
    PAUSE
    IF (SENSE SWITCH 2) 21,5
20 TYPE 37
    TYPE 34,I
    PAUSE
    GO TO 21
END
```

TABLE XXX—THERMODYNAMIC PROPERTIES OF H₂ (GAS)

[Molecular weight, 2.016]

T (°K)	C _p (cal mole °K)	H ₂ -H ₀ (kcal mole)	H ₂ (kcal mole)	S ₀ (cal mole °K)	$\frac{\Delta H^\circ}{RT}$	$\ln\left(-\frac{\Delta H^\circ}{RT}\right) = \frac{-\Delta T}{100}\left(\frac{a}{T} + b\right)$		log K	$\delta \log K = \frac{-\delta T}{T_0}\left(\frac{c}{T} + d\right)$	
						a	b		c	d
0	0	67.4169
298.16	6.892	2.0208	69.4407	31.211	175.8297	71.2998
300	6.895	2.0365	69.4344	31.224	174.7610	70.7414
400	6.974	2.7310	70.1179	33.250	141.1465	51.7421
500	6.954	3.4255	70.8064	34.869	105.4511	40.3099
600	7.008	4.1286	71.5155	36.081	88.1261	32.6660
700	7.078	4.8415	72.2484	37.167	75.7451	27.1921
800	7.078	5.574	72.9513	38.108	66.4582	23.0744
900	7.120	6.2840	73.6219	38.936	59.2022	19.8636
1000	7.130	6.9658	74.2827	39.709	53.4178	0.02806	17.2883	2291	0.08007
1100	7.100	7.6023	75.0092	40.2663	48.7111	4712	0.02453	15.1755	2987	0.02563
1200	7.107	8.2081	75.8150	41.045	44.7599	4318	0.02556	13.4165	1916	0.0315
1300	7.150	8.7739	76.5908	41.634	41.4128	3985	0.02637	11.9135	1772	0.02629
1400	7.165	9.3601	77.3470	42.1908	38.5100	3700	0.02653	10.6278	1648	0.01833
1500	7.222	10.0669	78.1138	42.7227	36.0168	3454	0.0265	9.5105	1541	0.01626
1600	7.282	11.4710	78.8009	43.2433	34.0620	3240	0.0272	8.5311	1447	0.01472
1700	7.329	12.2613	79.6782	43.7016	31.9311	3051	0.0270	7.6532	1361	0.01372
1800	8.0185	13.0581	80.4753	44.1571	30.2121	2884	0.0261	6.8911	1294	0.01173
1900	8.1063	13.8618	81.2817	44.5941	28.6716	2734	0.02170	6.2029	1225	0.0160
2000	8.159	14.6800	82.0669	45.0112	27.2829	2600	0.0231	5.5798	1166	0.0106
2100	8.222	15.5006	82.9265	45.4140	26.0215	2478	0.01954	5.0151	1112	0.00965
2200	8.277	16.3351	83.7520	45.7938	24.8786	2367	0.01867	4.5010	1063	0.00794
2300	8.324	17.1741	84.5610	46.1728	23.8408	2267	0.01782	4.0300	1018	0.00733
2400	8.377	18.0204	85.3473	46.5529	22.8987	2174	0.01660	3.5994	978	0.00640
2500	8.397	18.8735	86.2004	46.8812	22.0622	2089	0.01604	3.2018	940	0.00586
2600	8.4280	19.7331	87.1500	47.2183	21.3027	2011	0.01519	2.8314	905	0.00541
2700	8.4806	20.5990	88.0160	47.5151	20.6027	1938	0.01466	2.4808	873	0.00481
2800	8.7179	21.4769	88.8878	47.8622	19.9699	1870	0.01417	2.1772	844	0.00441
2900	8.8432	22.3685	89.7551	48.1702	19.3999	1807	0.01377	1.8821	815	0.00403
3000	8.887	23.2317	90.6086	48.4606	18.8808	1748	0.01323	1.6061	789	0.00368
3100	8.9118	24.1262	91.5371	48.7369	17.8437	1683	0.01291	1.3482	764	0.00335
3200	8.9366	25.0110	92.5309	49.0117	17.3017	1630	0.01281	1.1039	741	0.00325
3300	9.0133	25.9129	93.5288	49.3213	16.7919	1591	0.01265	.8781	719	0.00313
3400	9.0669	26.8168	94.2337	49.5911	16.3113	1546	0.01219	.6835	699	0.00279
3500	9.1125	27.7256	95.1425	49.8515	15.8574	1502	0.01208	.4610	680	0.00211
3600	9.1692	28.6392	96.0561	50.1119	15.4281	1461	0.01181	.6.2667	663	0.00228
3700	9.2070	29.5576	96.9753	50.3635	15.0214	1423	0.01153	-.0885	644	0.00224
3800	9.2529	30.4806	97.8975	50.6097	14.6351	1386	0.01132	-.2832	628	0.00197
3900	9.2979	31.4081	98.8250	50.8506	14.2687	1351	0.01125	-.2462	613	0.00175
4000	9.3421	32.3401	99.7570	51.0866	13.9197	1318	0.01104	-.4012	598	0.00165
4100	9.3856	33.2765	100.6934	51.3178	13.5872	1287	0.01067	-.5487	584	0.00145
4200	9.4284	34.2172	101.6341	51.5445	13.2701	1257	0.01057	-.6892	571	0.00141
4300	9.4704	35.1621	102.5760	51.7668	12.9672	1229	0.01058	-.8293	558	0.00118
4400	9.5118	36.1113	103.5282	51.9850	12.6775	1201	0.01031	-.8513	546	0.00097
4500	9.5526	37.0645	104.4814	52.1992	12.4003	1175	0.01017	-1.0736	535	0.00080
4600	9.5928	38.0217	105.4389	52.4096	12.1347	1150	0.01002	-1.1907	524	0.00071
4700	9.6324	38.9830	106.3999	52.6164	11.8800	1127	0.00971	-1.3029	514	0.00042
4800	9.6711	39.9482	107.3651	52.8196	11.6355	1104	0.00969	-1.4164	503	0.00045
4900	9.7099	40.9173	108.3342	53.0191	11.4005	1082	0.00950	-1.5135	494	0.00030
5000	9.7479	41.8901	109.3070	53.2159	11.1736	1061	0.00936	-1.6126	484	0.00030
5100	9.7853	42.8668	110.2837	53.4093	10.9572	1041	0.00931	-1.7077	475	0.00018
5200	9.8222	43.8472	111.2641	53.5997	10.7577	1021	0.00916	-1.7992	466	0.00018
5300	9.8586	44.8312	112.2481	53.7871	10.5644	1003	0.00893	-1.8873	458	0.0001
5400	9.8945	45.8189	113.2358	53.9717	10.3811	985	0.00891	-1.9731	450	0.0002
5500	9.9299	46.8101	114.2270	54.1536	10.1631	967	0.00862	-2.0539	442	0.00013
5600	9.9649	47.8048	115.2217	54.3328	9.9816	951	0.00876	-2.1327	434	0.00014
5700	9.9994	48.8031	116.2200	54.5095	9.8070	934	0.00867	-2.2087	427	0.00012
5800	10.0334	49.8017	117.2216	54.6837	9.6393	919	0.00854	-2.2822	420	0.00029
5900	10.0669	50.8007	118.2256	54.8555	9.4720	904	0.00843	-2.3531	413	0.00033
6000	10.1001	51.8181	119.2350	55.0250	9.3129	-2.4216

TABLE XLIV--THERMODYNAMIC PROPERTIES OF O_2 (GAS)

(Molecular weight, 32.0000)

T (°K)	C_p (cal mole °K)	$H_2^0 - H_2$ (kcal mole)	H_2^0 (kcal mole)	S_2^0 (cal mole °K)	$-\Delta H^0$ RT	$\ln \left(-\frac{\Delta H^0}{RT} \right) - \frac{-\Delta T}{100} \left(\frac{a}{T} + b \right)$		$\ln K'$	$\ln K = -\frac{\Delta T}{100} \left(\frac{a}{T} + d \right)$	
						a	b		c	d
0	0	2.0362
258.16	7.021	2.0747	4.1109	49.011	192.6835	80.0182
300	7.029	2.0826	4.1236	49.076	190.5635	81.0807
400	7.196	2.1927	4.8339	61.066	149.2649	58.5109
500	7.431	3.3288	6.3650	62.728	119.7013	45.5311
600	7.670	6.3263	54.105	99.9669	36.6260
700	7.883	5.0620	7.0682	55.303	85.8510	30.6499
800	8.063	5.8366	7.8558	56.368	75.2196	25.1854
900	8.212	6.7637	8.7669	57.327	66.9937	22.3515
1000	8.336	7.5012	9.5374	58.190	60.3812	0.02853	19.4490	2601	0.01823
1100	8.439	8.3100	10.3762	58.993	51.9651	0.03117	17.0545	2370	0.01550
1200	8.527	9.1884	11.2215	59.761	50.1179	0.03061	15.0640	2173	0.01322
1300	8.604	10.0108	12.0810	60.4220	46.6219	0.0373	13.3777	2000	0.01200
1400	8.674	10.7587	12.9449	61.0622	43.3966	0.0370	11.9307	1867	0.01083
1500	8.738	11.5753	13.8155	61.6828	40.4926	0.0362	10.6752	1744	0.00960
1600	8.800	12.3562	14.6924	62.2287	37.9993	0.0357	9.5756	1637	0.00826
1700	8.858	13.1091	15.5753	62.7040	35.7976	0.0351	8.6044	1542	0.00733
1800	8.916	13.8278	16.4640	63.2719	33.8787	0.0347	7.7463	1458	0.00663
1900	8.973	14.5223	17.3585	63.7585	32.0845	0.0340	6.9655	1383	0.00550
2000	9.029	15.2224	18.2586	64.2172	30.5043	0.0336	6.2665	1315	0.00491
2500	9.684	17.1260	19.1644	64.6500	26.0733	0.03156	5.6384	1253	0.00455
3000	9.739	18.0892	20.0754	65.0829	27.7711	0.0323	5.0613	1197	0.00407
3500	9.794	18.9658	20.9620	65.5064	26.5869	0.0288	4.5308	1146	0.00370
4000	9.848	19.7779	21.9141	65.8828	25.4889	0.0200	4.0586	1099	0.00300
4500	9.901	20.5054	22.8416	66.2614	21.4533	0.0101	3.6187	1056	0.00265
5000	9.954	21.7381	23.7743	66.6272	23.5510	0.0120	3.2060	1016	0.00230
5500	9.995	22.6761	24.7123	66.9812	22.6928	0.01060	2.8277	980	0.00210
6000	9.955	23.6191	25.6553	67.3241	21.8922	0.00979	2.4756	945	0.00201
6500	9.963	24.5670	26.6052	67.6568	21.1462	0.00913	2.1477	913	0.00187
7000	9.951	25.5197	27.5559	67.9797	20.4494	0.00831	1.8415	883	0.00166
7500	9.996	26.4770	28.5132	68.2936	19.7969	0.00781	1.5550	855	0.00161
8000	9.940	27.4388	29.4750	68.5990	19.1846	0.0071	1.2862	829	0.00139
8500	9.982	28.4049	30.4411	68.8963	18.6091	0.00622	1.0337	801	0.00123
9000	9.724	29.3752	31.4114	69.1859	18.0670	0.00540	0.7960	781	0.00106
9500	9.762	30.3494	32.3856	69.4683	17.5536	0.00469	.5718	759	0.00097
10000	9.799	31.3275	33.3637	69.7459	17.0724	0.00420	0.3690	739	0.00077
10500	9.835	32.3092	34.3454	70.0128	16.6148	0.00350	.1595	719	0.00069
11000	9.869	33.2914	35.3296	70.2756	16.1813	0.00278	-.0304	700	0.00071
11500	9.901	34.2829	36.3191	70.5323	15.7698	0.00225	-.2106	682	0.00070
12000	9.932	35.2745	37.3107	70.7834	15.3788	0.00161	-.3818	665	0.00070
12500	9.960	36.2691	38.3053	71.0290	15.0067	0.00107	-.5447	649	0.00068
13000	9.987	37.2665	39.3027	71.2693	14.6524	0.00069	-.6990	634	0.00059
13500	10.013	38.2665	40.3027	71.5046	14.3144	0.0010	-.8479	619	0.00062
14000	10.037	39.2690	41.3052	71.7351	13.9918	0.0014	-.9922	605	0.00043
14500	10.060	40.2738	42.3100	71.9609	13.6835	0.00063	-.1.1243	592	0.00050
15000	10.081	41.2809	43.3171	72.1822	13.3887	0.00089	-.1.2515	579	0.00051
15500	10.102	42.2901	44.3263	72.3966	13.1064	0.00127	-.1.3772	567	0.00048
16000	10.121	43.3013	45.3373	72.6122	12.8360	0.00162	-.1.4958	555	0.00053
16500	10.139	44.3143	46.3465	72.8210	12.5766	0.00190	-.1.6066	543	0.00049
17000	10.156	45.3290	47.3532	73.0261	12.3277	0.00208	-.1.7188	533	0.00049
17500	10.172	46.3454	48.3616	73.2273	12.0886	0.00232	-.1.8238	522	0.00062
18000	10.187	47.3634	49.3696	73.4250	11.8588	0.00240	-.1.9248	512	0.00060
18500	10.201	48.3828	50.4190	73.6192	11.6378	0.00248	-.2.0220	502	0.00064
19000	10.215	49.4030	51.4398	73.8100	11.4251	0.00252	-.2.1156	493	0.00059
19500	10.228	50.4257	52.4619	73.9978	11.2201	0.00286	-.2.2058	484	0.00057
20000	10.239	51.4455	53.4858	74.1819	11.0226	0.00228	-.2.2928	475	0.00067
20500	10.250	52.4735	54.5097	74.3632	10.8322	0.00316	-.2.3758	466	0.00077
21000	10.261	53.4991	55.5353	74.5416	10.6483	0.00335	-.2.4579	458	0.00077
21500	10.271	54.5250	56.5618	74.7171	10.4700	0.00343	-.2.5363	450	0.00080
22000	10.279	55.5531	57.5893	74.8896	10.2995	0.00355	-.2.6131

TABLE XXXIII—THERMODYNAMIC PROPERTIES OF H₂O (GAS)

59

[Molecular weight, 18.016]

T (°K)	C _p ($\frac{\text{cal}}{\text{mole} \cdot ^\circ\text{K}}$)	$H_f^\circ - H_f^\circ$ ($\frac{\text{cal}}{\text{mole}}$)	H_f° ($\frac{\text{cal}}{\text{mole}}$)	Δ_f° ($\frac{\text{cal}}{\text{mole} \cdot ^\circ\text{K}}$)	$-\frac{\Delta_f^\circ}{RT}$	$\ln K = -\frac{\Delta_f^\circ}{RT} - \frac{\Delta_f^\circ}{100} \left(\frac{1}{T} + \frac{1}{T^2} \right)$		$\ln K = -\frac{\Delta_f^\circ}{RT} - \frac{\Delta_f^\circ}{100} \left(\frac{1}{T} + \frac{1}{T^2} \right)$	
						a	b	c	d
0	0	0	11.3411	45.106	273.2200	151.5648
25	8.025	2.3677	13.7088	45.151	270.9541	160.5708
50	8.185	3.1940	14.5251	47.490	270.0566	110.2372
75	8.315	4.0255	15.3566	49.344	273.9534	85.9609
100	8.427	4.8822	16.2133	50.903	187.7653	69.7280
125	8.509	5.7715	17.1026	52.269	199.8693	58.0546
150	8.571	6.6866	18.0207	53.490	111.1213	49.3548
175	8.615	7.6347	18.9658	54.589	125.7485	42.8361
200	8.661	8.6080	19.9391	55.6183	119.4355	11.015	0.07316	37.0674	4875
225	10.115	9.6083	20.9391	56.5712	109.3187	10.019	0.06833	32.5840	4439
250	10.113	10.6362	21.9673	57.4654	94.9012	9.188	0.06491	28.8369	4076
275	10.088	11.6962	23.0213	58.2959	87.7986	8.496	0.06197	25.6655	3798
300	10.049	12.7691	24.1092	59.1084	81.6758	7.880	0.05966	22.9395	3505
325	10.001	13.8712	25.2026	59.8987	76.3045	7.366	0.05318	20.5727	3276
350	11.343	14.9651	26.3262	60.5939	71.7016	6.913	0.04853	18.4983	3075
375	11.534	16.1889	27.4700	61.2873	67.5806	6.514	0.04491	16.6852	2898
400	11.708	17.3910	28.6321	61.9515	63.9267	6.160	0.03959	15.0332	2741
425	11.865	18.4767	29.8108	62.5887	60.6180	5.843	0.03506	13.5710	2600
450	12.008	19.6733	31.0444	63.2010	57.6676	5.557	0.03271	12.2533	2474
475	12.148	20.8806	32.3117	63.7900	55.0687	5.299	0.02966	11.0505	2359
500	12.256	22.1063	33.6314	64.3574	52.5794	5.064	0.02686	9.9550	2255
525	12.364	23.3513	34.9934	64.9045	50.3118	4.849	0.02468	8.9798	2160
550	12.463	24.6727	36.4038	65.4328	48.2667	4.653	0.02220	8.0953	2072
575	12.553	25.8235	37.7546	65.9434	46.4133	4.471	0.02049	7.2289	1991
600	12.638	27.0831	39.4142	66.4374	44.6732	4.304	0.01893	6.4632	1916
625	12.718	28.3568	40.8192	66.9159	43.0465	4.149	0.01791	5.7943	1846
650	12.790	29.6659	42.1699	67.3796	41.5318	4.005	0.01717	5.1971	1781
675	12.852	30.9677	43.5271	67.8298	40.1163	3.871	0.01607	4.6434	1721
700	12.913	32.1650	44.8211	68.2601	38.8049	3.747	0.01509	4.1261	1666
725	12.968	33.4960	46.0211	68.6804	37.6098	3.630	0.01413	3.6370	1613
750	13.018	34.7893	47.1204	69.1029	36.5303	3.520	0.01330	3.1790	1561
775	13.064	36.0631	48.1245	69.5642	35.4717	3.417	0.01256	2.7555	1511
800	13.107	37.3020	49.7391	69.8949	34.4308	3.320	0.01193	2.3729	1463
825	13.147	38.7147	50.0498	70.2764	33.4137	3.228	0.01136	1.9458	1417
850	13.184	40.0612	51.5023	70.6463	32.5136	3.142	0.01081	1.6022	1372
875	13.218	41.3634	52.1821	71.0080	31.6884	3.060	0.01036	1.301	1325
900	13.250	42.6747	53.4658	71.3649	30.8779	2.981	0.01004	1.038	1280
925	13.280	43.6612	54.3324	71.7054	30.1087	2.907	0.01025	0.8162	1237
950	13.308	45.3666	55.6617	72.0420	29.3777	2.836	0.01079	0.6372	1195
975	13.334	46.6627	57.0638	72.3710	28.6822	2.769	0.01021	0.4945	1156
1000	13.358	47.9573	58.5281	72.6926	28.0197	2.705	0.00983	0.3812	1118
1025	13.381	49.3243	60.0556	73.0071	27.3875	2.643	0.00977	0.2943	1084
1050	13.403	50.7742	62.0453	73.3150	26.7843	2.584	0.00986	0.2337	1051
1075	13.424	52.0148	63.7459	73.6164	26.2079	2.528	0.00994	0.1933	1019
1100	13.444	53.5582	65.4893	73.9117	25.6593	2.473	0.00993	0.1609	989
1125	13.464	54.7036	66.0347	74.2011	25.1281	2.421	0.01019	0.1350	961
1150	13.481	56.0510	67.5821	74.4817	24.6218	2.371	0.01012	0.1131	935
1175	13.502	57.3602	68.7313	74.7625	24.1361	2.323	0.01070	0.0930	910
1200	13.521	58.7114	70.0825	75.0359	23.6698	2.276	0.01063	0.0746	886
1225	13.540	60.1044	71.4555	75.3058	23.2217	2.232	0.01077	0.0581	861
1250	13.559	61.4594	72.7903	75.5699	22.7937	2.188	0.01088	0.0432	837
1275	13.577	62.8402	74.1473	75.8254	22.3766	2.148	0.01072	0.0315	813
1300	13.596	64.1748	75.5059	76.0794	21.9765	2.108	0.01063	0.0226	790
1325	13.614	65.5553	76.8694	76.3250	21.5916	2.070	0.01069	0.0160	767
1350	13.633	66.8977	78.2283	76.5745	21.2203	2.033	0.01063	0.0110	745
1375	13.651	68.2619	79.5930	76.8159	20.8620	1.998	0.01062	0.0080	723
1400	13.669	69.6279	80.9590	77.0535	20.5159	1.963	0.01069	0.0060	701
1425	13.687	70.9957	82.3288	77.2879	20.1816	1.930	0.01088	0.0040	679
1450	13.705	72.3653	83.6994	77.5176	19.8585	0.0020	657

GENERAL METHOD AND TABLES FOR COMPUTATION OF EQUILIBRIUM COMPOSITION AND TEMPERATURE

TABLE XLIII—THERMODYNAMIC PROPERTIES OF O (GAS)

[Atomic weight, 16.0000]

T (°K)	C_p ($\frac{\text{cal}}{\text{mole} \cdot ^\circ\text{K}}$)	$H_f - H_0$ ($\frac{\text{cal}}{\text{mole}}$)	H_f ($\frac{\text{kcal}}{\text{mole}}$)	S_f ($\frac{\text{cal}}{\text{mole} \cdot ^\circ\text{K}}$)
0	0	50.9011
200.16	5.2961	1.4974	51.3115	38.4690
300	5.2538	1.6170	51.3211	38.8010
400	5.1411	2.1319	51.7490	39.9915
500	5.0802	2.6454	52.2495	41.1908
600	5.0486	3.1517	52.7528	42.0540
700	5.0281	3.6535	53.2596	42.8307
800	5.0150	4.1576	53.7617	43.5611
900	5.0055	4.6587	54.2628	44.0914
1000	4.9988	5.1588	54.7629	44.6183
1100	4.9936	5.6584	55.2625	45.0945
1200	4.9894	6.1576	55.7617	45.5288
1300	4.9864	6.6564	56.2605	45.9281
1400	4.9838	7.1549	56.7580	46.2977
1500	4.9819	7.6532	57.2573	46.6413
1600	4.9805	8.1513	57.7554	46.9726
1700	4.9792	8.6493	58.2534	47.2916
1800	4.9781	9.1471	58.7512	47.5992
1900	4.9778	9.6450	59.2491	47.8984
2000	4.9776	10.1427	59.7468	48.1937
2100	4.9778	10.6405	70.2446	48.5165
2200	4.9784	11.1383	70.7424	48.8481
2300	4.9796	11.6362	71.2403	49.1845
2400	4.9812	12.1343	71.7384	49.5854
2500	4.9834	12.6325	72.2366	49.9818
2600	4.9862	13.1310	72.7351	49.3803
2700	4.9897	13.6298	73.2339	49.3696
2800	4.9935	14.1289	73.7330	49.7501
2900	4.9986	14.6285	74.2326	49.8254
3000	5.0041	15.1287	74.7328	50.9050
3100	5.0102	15.6294	75.2335	50.2592
3200	5.0170	16.1307	75.7348	50.4183
3300	5.0245	16.6328	76.2369	50.5728
3400	5.0325	17.1357	76.7398	50.7229
3500	5.0411	17.6393	77.2434	50.8659
3600	5.0502	18.1439	77.7480	51.0111
3700	5.0599	18.6494	78.2535	51.1496
3800	5.0700	19.1559	78.7590	51.2846
3900	5.0805	19.6634	79.2675	51.4165
4000	5.0914	20.1720	79.7761	51.5452
4100	5.1026	20.6817	80.2858	51.6711
4200	5.1140	21.1925	80.7965	51.7942
4300	5.1257	21.7045	81.3086	51.9147
4400	5.1375	22.2177	81.8216	52.0322
4500	5.1495	22.7320	82.3361	52.1483
4600	5.1616	23.2476	82.8517	52.2615
4700	5.1738	23.7644	83.3685	52.3727
4800	5.1860	24.2824	83.8865	52.4817
4900	5.1981	24.8016	84.4057	52.5888
5000	5.2102	25.3220	84.9261	52.6939
5100	5.2223	25.8436	85.4477	52.7972
5200	5.2344	26.3664	85.9705	52.8988
5300	5.2464	26.8905	86.4945	52.9966
5400	5.2583	27.4157	87.0198	53.0903
5500	5.2701	27.9421	87.5462	53.1813
5600	5.2818	28.4697	88.0738	53.2684
5700	5.2933	28.9985	88.6025	53.3520
5800	5.3047	29.5294	89.1323	53.4742
5900	5.3159	30.0594	89.6633	53.5940
6000	5.3270	30.5916	90.1957	53.6644

TABLE XXIX—THERMODYNAMIC PROPERTIES OF H (GAS)

91

[Atomic weight, 1.008]

T (°K)	C_p ($\frac{\text{cal}}{\text{mole} \cdot ^\circ\text{K}}$)	$H_f - H_g$ ($\frac{\text{cal}}{\text{mole}}$)	H_f ($\frac{\text{cal}}{\text{mole}}$)	S_f ($\frac{\text{cal}}{\text{mole} \cdot ^\circ\text{K}}$)
0	-----	0	85.3285	-----
25, 16	4.0680	1.4812	86.8097	27.3927
300	4.0680	1.4901	86.8153	27.4253
400	4.0680	1.4972	87.8157	28.8524
500	4.0680	2.4810	87.8125	29.0010
600	4.0680	2.9608	88.3093	30.8907
700	4.0680	3.4775	88.8061	31.0325
800	4.0680	3.9711	89.3029	32.2050
900	4.0680	4.4712	89.7997	32.8811
1000	4.0680	4.9680	90.2965	33.4045
1100	4.0680	5.4618	90.7933	33.8780
1200	4.0680	5.9516	91.2901	34.3103
1300	4.0680	6.4381	91.7869	34.7079
1400	4.0680	6.9252	92.2837	35.0761
1500	4.0680	7.4120	92.7805	35.4188
1600	4.0680	7.8988	93.2773	35.7395
1700	4.0680	8.3856	93.7741	36.0407
1800	4.0680	8.8724	94.2709	36.3216
1900	4.0680	9.3592	94.7677	36.5932
2000	4.0680	9.8460	95.2645	36.8480
2100	4.0680	10.3328	95.7613	37.0904
2200	4.0680	10.8196	96.2581	37.3215
2300	4.0680	11.3064	96.7549	37.5424
2400	4.0680	11.7932	97.2517	37.7538
2500	4.0680	12.2800	97.7485	37.9560
2600	4.0680	12.7668	98.2453	38.1515
2700	4.0680	13.2536	98.7421	38.3390
2800	4.0680	13.7404	99.2389	38.5106
2900	4.0680	14.2272	99.7357	38.6640
3000	4.0680	14.7140	100.2325	38.8024
3100	4.0680	15.2008	100.7293	39.0253
3200	4.0680	15.6876	101.2261	39.1830
3300	4.0680	16.1744	101.7229	39.3350
3400	4.0680	16.6612	102.2197	39.4842
3500	4.0680	17.1480	102.7165	39.6282
3600	4.0680	17.6348	103.2133	39.7681
3700	4.0680	18.1216	103.7101	39.9043
3800	4.0680	18.6084	104.2069	40.0358
3900	4.0680	19.0952	104.7037	40.1658
4000	4.0680	19.5820	105.2005	40.2916
4100	4.0680	20.0688	105.6973	40.4142
4200	4.0680	20.5556	106.1941	40.5340
4300	4.0680	21.0424	106.6909	40.6509
4400	4.0680	21.5292	107.1877	40.7651
4500	4.0680	22.0160	107.6845	40.8767
4600	4.0680	22.5028	108.1813	40.9850
4700	4.0680	22.9896	108.6781	41.0925
4800	4.0680	23.4764	109.1749	41.1973
4900	4.0680	23.9632	109.6717	41.2998
5000	4.0680	24.4500	110.1685	41.4002
5100	4.0680	24.9368	110.6653	41.4985
5200	4.0680	25.4236	111.1621	41.5950
5300	4.0680	25.9104	111.6589	41.6893
5400	4.0680	26.3972	112.1557	41.7825
5500	4.0680	26.8840	112.6525	41.8738
5600	4.0680	27.3708	113.1493	41.9632
5700	4.0680	27.8576	113.6461	42.0511
5800	4.0680	28.3444	114.1429	42.1376
5900	4.0680	28.8312	114.6397	42.2224
6000	4.0680	29.3180	115.1365	42.3059

GENERAL METHOD AND TABLES FOR COMPUTATION OF EQUILIBRIUM COMPOSITION AND TEMPERATURE

TABLE XIV—THERMODYNAMIC PROPERTIES OF OH (GAS)

[Molecular weight, 17.008]

62

T (°K)	C _p (cal mole °K)	H _f -H ₀ (kcal mole)	H _f (kcal mole)	S _f (cal mole °K)	-ΔH° RT	ln(-ΔH°/RT) = -ΔT(1/T + 1/T°)		ln K	ln K = -ΔT(1/T + 1/T°)	
						a	b		c	d
298.16	7.141	0	41.7266	43.888	176.7827
300	7.139	2.1002	46.8428	43.931	169.7365	00.3677
400	7.071	2.8296	47.5562	45.978	127.6916	58.9110
500	7.018	3.5559	48.2616	47.559	102.4572	50.4585
600	7.073	4.2808	48.9671	48.810	85.6993	39.3522
700	7.087	4.9959	49.6725	49.927	72.6991
800	7.101	5.6984	50.3779	50.877	61.5888	31.7270
900	7.114	6.3874	51.0832	51.723	51.5982	26.1657
1000	7.127	7.0690	51.7886	52.4910	43.9464	22.6043
1100	7.140	7.7436	52.4939	53.1919	37.9119	4.575	0.02600	19.4813
1200	7.153	8.4119	53.1992	53.8170	32.5901	4.191	0.02615	16.9901	2.227	0.02615
1300	7.166	9.0739	53.8205	54.3556	27.8118	3.873	0.02777	14.9207	3029	0.02157
1400	7.179	9.7296	54.3512	54.8078	23.4566	3.599	0.02917	13.2113	1473	0.02172
1500	7.192	10.3790	54.8019	55.2675	19.4052	3.361	0.03047	11.7583	1723	0.01600
1600	7.205	11.0211	55.2675	55.7359	15.6259	3.153	0.03167	10.5967	1698	0.01675
1700	7.218	11.6559	55.7359	56.2098	12.1935	2.970	0.03280	9.4213	1494	0.01535
1800	7.231	12.2834	56.2098	56.6899	9.0217	2.810	0.03382	8.4687	1407	0.01535
1900	7.244	12.9039	56.6899	57.1654	6.2268	2.668	0.03471	7.6295	1327	0.01194
2000	7.257	13.5174	57.1654	57.6371	3.7414	2.543	0.03549	6.8753	1255	0.01087
2100	7.270	14.1239	57.6371	58.1049	1.5699	2.433	0.03617	6.2079	1190	0.01000
2200	7.283	14.7234	58.1049	58.5687	2.335	0.03675	5.6127	1132	0.00904
2300	7.296	15.3159	58.5687	59.0287	2.245	0.03723	5.0842	1080	0.00849
2400	7.309	15.9014	59.0287	59.4849	2.160	0.03771	4.6149	1032	0.00790
2500	7.322	16.4799	59.4849	59.9371	2.080	0.03819	4.1983	990	0.00730
2600	7.335	17.0514	59.9371	60.3859	2.005	0.03867	3.8292	949	0.00670
2700	7.348	17.6159	60.3859	60.8307	1.935	0.03915	3.5037	912	0.00603
2800	7.361	18.1734	60.8307	61.2714	1.870	0.03963	3.2163	878	0.00541
2900	7.374	18.7239	61.2714	61.7087	1.809	0.04011	2.9619	848	0.00484
3000	7.387	19.2674	61.7087	62.1429	1.752	0.04059	2.7344	817	0.00430
3100	7.400	19.8039	62.1429	62.5739	1.699	0.04107	2.5319	790	0.00377
3200	7.413	20.3334	62.5739	63.0014	1.650	0.04155	2.3514	764	0.00325
3300	7.426	20.8559	63.0014	63.4259	1.604	0.04203	2.1909	740	0.00273
3400	7.439	21.3714	63.4259	63.8474	1.561	0.04251	2.0474	718	0.00221
3500	7.452	21.8799	63.8474	64.2659	1.520	0.04299	1.9189	697	0.00170
3600	7.465	22.3814	64.2659	64.6814	1.481	0.04347	1.8014	677	0.00118
3700	7.478	22.8759	64.6814	65.0939	1.443	0.04395	1.6939	659	0.00066
3800	7.491	23.3634	65.0939	65.5034	1.407	0.04443	1.5964	641	0.00014
3900	7.504	23.8439	65.5034	65.9099	1.373	0.04491	1.5089	624	0.00000
4000	7.517	24.3174	65.9099	66.3134	1.340	0.04539	1.4314	608	0.00000
4100	7.530	24.7839	66.3134	66.7139	1.308	0.04587	1.3639	593	0.00000
4200	7.543	25.2434	66.7139	67.1114	1.277	0.04635	1.3064	579	0.00000
4300	7.556	25.6959	67.1114	67.5059	1.247	0.04683	1.2589	565	0.00000
4400	7.569	26.1414	67.5059	67.8974	1.218	0.04731	1.2214	551	0.00000
4500	7.582	26.5799	67.8974	68.2859	1.190	0.04779	1.1839	538	0.00000
4600	7.595	27.0114	68.2859	68.6714	1.163	0.04827	1.1464	525	0.00000
4700	7.608	27.4359	68.6714	69.0539	1.137	0.04875	1.1089	512	0.00000
4800	7.621	27.8534	69.0539	69.4334	1.112	0.04923	1.0714	500	0.00000
4900	7.634	28.2639	69.4334	69.8099	1.088	0.04971	1.0339	488	0.00000
5000	7.647	28.6674	69.8099	70.1834	1.064	0.05019	0.9964	476	0.00000
5100	7.660	29.0639	70.1834	70.5539	1.041	0.05067	0.9589	464	0.00000
5200	7.673	29.4534	70.5539	70.9214	1.018	0.05115	0.9214	452	0.00000
5300	7.686	29.8359	70.9214	71.2859	0.996	0.05163	0.8839	440	0.00000
5400	7.699	30.2114	71.2859	71.6474	0.974	0.05211	0.8464	428	0.00000
5500	7.712	30.5799	71.6474	72.0059	0.953	0.05259	0.8089	416	0.00000
5600	7.725	30.9414	72.0059	72.3614	0.932	0.05307	0.7714	404	0.00000
5700	7.738	31.2959	72.3614	72.7139	0.911	0.05355	0.7339	392	0.00000
5800	7.751	31.6434	72.7139	73.0634	0.891	0.05403	0.6964	380	0.00000
5900	7.764	31.9839	73.0634	73.4099	0.871	0.05451	0.6589	368	0.00000
6000	7.777	32.3174	73.4099	73.7534	0.851	0.05499	0.6214	356	0.00000
6100	7.790	32.6439	73.7534	74.0939	0.831	0.05547	0.5839	344	0.00000
6200	7.803	32.9634	74.0939	74.4314	0.811	0.05595	0.5464	332	0.00000
6300	7.816	33.2759	74.4314	74.7659	0.791	0.05643	0.5089	320	0.00000
6400	7.829	33.5814	74.7659	75.0974	0.771	0.05691	0.4714	308	0.00000
6500	7.842	33.8799	75.0974	75.4259	0.751	0.05739	0.4339	296	0.00000
6600	7.855	34.1714	75.4259	75.7514	0.731	0.05787	0.3964	284	0.00000
6700	7.868	34.4559	75.7514	76.0739	0.711	0.05835	0.3589	272	0.00000
6800	7.881	34.7334	76.0739	76.3934	0.691	0.05883	0.3214	260	0.00000
6900	7.894	35.0039	76.3934	76.7099	0.671	0.05931	0.2839	248	0.00000
7000	7.907	35.2674	76.7099	77.0234	0.651	0.05979	0.2464	236	0.00000
7100	7.920	35.5239	77.0234	77.3339	0.631	0.06027	0.2089	224	0.00000
7200	7.933	35.7734	77.3339	77.6414	0.611	0.06075	0.1714	212	0.00000
7300	7.946	36.0159	77.6414	77.9459	0.591	0.06123	0.1339	200	0.00000
7400	7.959	36.2514	77.9459	78.2474	0.571	0.06171	0.0964	188	0.00000
7500	7.972	36.4799	78.2474	78.5459	0.551	0.06219	0.0589	176	0.00000
7600	7.985	36.7014	78.5459	78.8414	0.531	0.06267	0.0214	164	0.00000
7700	7.998	36.9159	78.8414	79.1339	0.511	0.06315	0.0000	152	0.00000
7800	8.011	37.1234	79.1339	79.4234	0.491	0.06363	140	0.00000
7900	8.024	37.3239	79.4234	79.7099	0.471	0.06411	128	0.00000
8000	8.037	37.5174	79.7099	80.0000	0.451	0.06459	116	0.00000